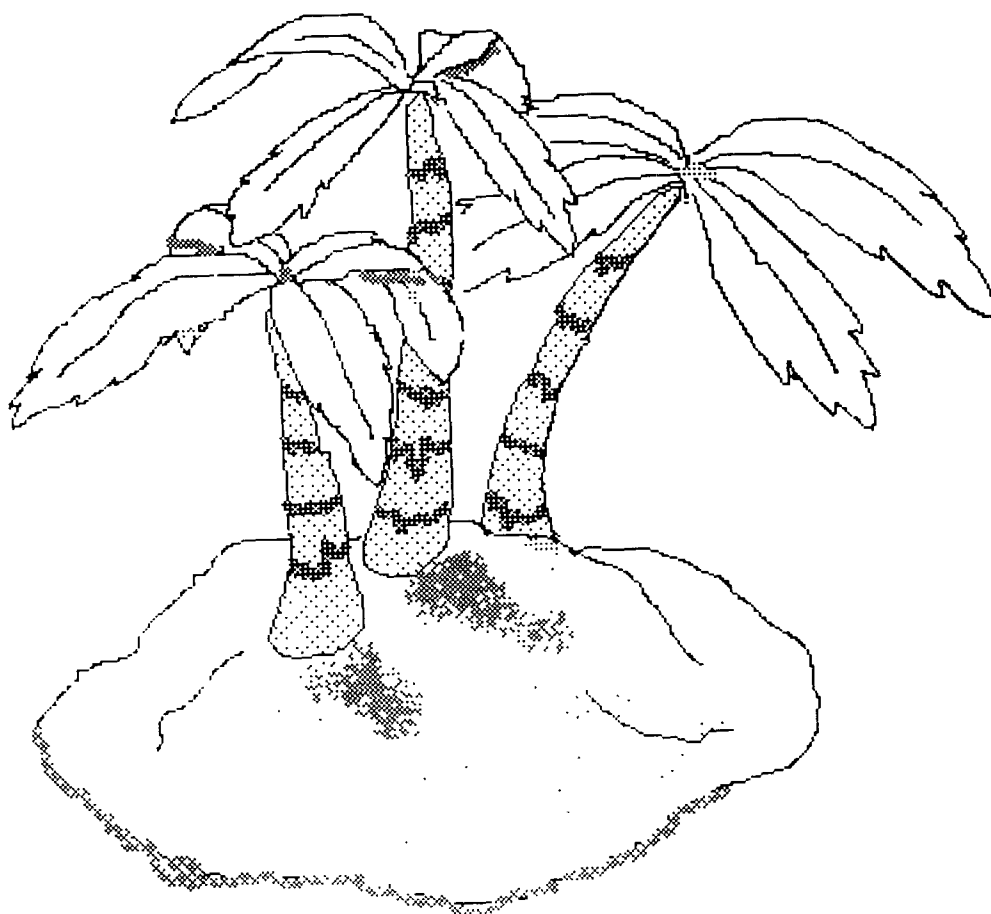




OASIS: Parameter Estimation System for Aquifer Restoration Models

User's Manual Version 2.0



EPA/600/8-90/039
February 1990

**OASIS: PARAMETER ESTIMATION SYSTEM
FOR AQUIFER RESTORATION MODELS
User's Manual Version 2.0**

by

Charles J. Newell
John F. Haasbeek
Loren P. Hopkins
Sarah E. Alder-Schaller
Hanadi S. Rifai
Philip B. Bedient
G. Anthony Gorry

Department of Environmental Science and Engineering
Rice University
P.O. Box 1892
Houston, Texas 77251-1892

CR-814495

Project Officer

J. R. Williams
Robert S. Kerr Environmental Research Laboratory
U.S. Environmental Protection Agency
Ada, Oklahoma 74820

ROBERT S. KERR ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ADA, OKLAHOMA 74820

DISCLAIMER

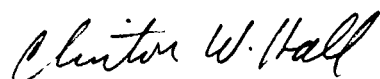
The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Assistance Agreement No. CR-814495 to Rice University. It has been subjected to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute an endorsement or recommendation for use.

FOREWORD

EPA is charged by Congress to protect the Nation's land, air and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and control of toxic substances, pesticides, noise and radiation, the agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil, and indigenous organisms; (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

This user's manual instructs the user in the execution of the software package OASIS, a decision support system for ground water contaminant modeling. This guide should give the user access to critical information for analyzing ground water contamination problems.



Clinton W. Hall
Director
Robert S. Kerr Environmental
Research Laboratory

ABSTRACT

OASIS, a decision support system for ground water contaminant modeling, has been developed for the EPA by Rice University, through the National Center for Ground Water Research. As a decision support system, OASIS was designed to provide a set of tools which will help scientists and modelers assess ground water contamination problems. OASIS is a graphical decision support system and was developed around BIOPLUME II (Rifai et al., 1988), a numerical model which simulates the aerobic degradation of dissolved hydrocarbons in ground water.

The OASIS system was developed in the HyperCard environment and, unlike traditional software, contains extensive documentation and help onscreen. Question mark icons throughout OASIS lead the user to further discussion and definitions, thereby allowing the system to be fully operational without the aid of paper documentation.

The information in OASIS includes documentation, a hydrogeologic database, two chemical databases, several simple hydrogeologic models, and the BIOPLUME II model with preprocessors and postprocessors. The system was developed for use on Macintosh personal computers and now contains over 1600 screens and 9 megabytes (Mb) of information. The installation of the software requires 10 Mb of disk space.

CONTENTS

Disclaimer	ii
Foreword	iii
Abstract	iv
Figures	vi
1.0 Introduction	1
2.0 HyperCard	3
3.0 OASIS System Contents	4
General Information	4
Notebook	8
Reference Library	8
Hydrogeologic Database	10
General Chemical Database	12
Specific Chemical Database	12
Darcy's Law	14
Analytical Models	14
BIOPLUME II Model	14
BIOPLUME II PreProcessor	15
Run Model	19
OASIS Example	20
4.0 OASIS System Requirements	24
5.0 Instructions for Installing the OASIS Software	25
6.0 OASIS Installation Procedure for Experienced Users	28
7.0 Using OASIS	30
8.0 General OASIS Exercises	31
9.0 BioGraph User's Manual	46
References	50
Software Disclaimer	51

FIGURES

<u>Number</u>		<u>Page</u>
1	The system outline card for OASIS	5
2	Card from the specific chemical database, benzene	6
3	Key to common button symbols and icons in OASIS	7
4	Flowchart from the source by industry reference stack	9
5	Decision process for selecting a hydrogeologic setting	11
6	Card from the general chemical database, benzene	13
7	First card from the BIOPLUME II preprocessor	16
8	Transmissivity card	18
9	Hydrogeologic setting card	21
10	Output from the BioGraph postprocessor	23

OASIS: PARAMETER ESTIMATION SYSTEM FOR AQUIFER RESTORATION MODELS

1.0 INTRODUCTION

OASIS, a decision support system for ground water contaminant modeling, has been developed for the EPA by Rice University, through the National Center for Ground Water Research. As a decision support system, OASIS was designed to provide scientists and modelers with a collection of tools to help assess and analyze ground water contamination problems. New types of software are being developed for problems that have traditionally been difficult to implement using conventional computer technology. Decision Support Systems (DSS) are a class of software that help people deal with broad problems that do not have a clearly defined solution procedure. The use of a ground water contaminant transport model is a semi-structured problem which requires the scientist to make a series of decisions related to representation of the site, application of available data, and types of simulations to be performed.

OASIS is a graphical decision support system and was developed around the BIOPLUME II model (Rifai et al., 1988). OASIS contains an extensive amount of information designed to facilitate the task of ground water modeling. The reference stack incorporated in the system contains libraries of information related to the field ground water. OASIS contains a general chemical database containing 117 chemicals, with one card of information per chemical, and a specific chemical database which contains 18 chemicals, with 25 cards of information per chemical. Also contained in OASIS is a hydrogeologic database, which was developed through an extensive technical survey of ground water professionals. Data from 400 field sites across the country was obtained from ground water professionals and incorporated into this database.

The OASIS system allows the user to perform three different levels of modeling. At the lowest level, the Darcy's law stack calculates the ground water velocity in a system where hydraulic conductivity, gradient, and porosity are known. At the next level, ODAST, (Javandel, Doughty, and Tsang, 1984), a one-dimensional solute transport model, considers advection, dispersion, solute decay, source decay, and adsorption in a ground water system. Finally, OASIS contains BIOPLUME II, a two-dimensional computer model that simulates the transport of dissolved hydrocarbons under the influence of oxygen-limited biodegradation. BIOPLUME II also simulates reaeration and anaerobic biodegradation as a first order decay in hydrocarbon concentrations.

Unlike traditional software, the OASIS system contains extensive documentation and help onscreen. Throughout the system, question mark icons lead the user to further discussion and definitions. Thus, the system has been designed to be fully operational without the aid of

paper documentation. The OASIS system was developed using HyperCard on Macintosh personal computers and now contains over 1600 screens and 9 megabytes (Mb) of information, thus requiring the use of a 20 Mb hard disk. It is noted that the installation of the software actually requires 10 Mb of disk space.

2.0 HYPERCARD®

OASIS was built using HyperCard, a software package provided with the Apple Macintosh. In the HyperCard environment, each different screen of information is called a "card," and cards are collected into groups called "stacks." The cards within a stack are connected to each other by "links." These links may take many forms. For example, a link may consist of a "button" which sends the user to a particular card or a "field" which displays data taken from another card. In HyperCard, fields and buttons link together cards, stacks, and other files and programs in the computer. The user is able to navigate through large amounts of information using a series of mouse clicks on active buttons. Thus, instead of going screen by screen through the computer (or similarly page by page in a book), a user is allowed nonsequential access to information in the system. The first card in the OASIS system (the OASIS Home card) contains an *Intro* button which gives more information about HyperCard. The user is also referred to the HyperCard user's manual for any additional questions.

3.0 OASIS SYSTEM CONTENTS

The OASIS system consists of documentation, a hydrogeologic database, two chemical databases, several simple hydrogeologic models, and the BIOPLUME II model with preprocessors and postprocessors. Figure 1 shows an overall outline of the system that is shown on the computer screen to users of OASIS. Each round rectangle is a "button" that the user can click on with the mouse to go to a particular part of the system.

General Information

Each card in OASIS consists of one screen of information on a picture background. Cards are organized into stacks of related information, with most cards in a stack having similar backgrounds. Several different backgrounds are used in the OASIS system. These backgrounds include pictures of tab cards, open books, notebooks, etc. The background of the card pictured in Figure 2, from the specific chemical database, is a spiral notebook.

Text in a card is entered into a text field. Text fields take many different forms: rectangular, opaque (on a white background), shadowed, transparent (only the text can be seen, not the field) or scrolling. In Figure 2, the physical data is entered into transparent fields, whereas the fire hazard data is entered into a scrolling field. In a scrolling field, all the information cannot be viewed at the same time, and to see additional information the user clicks the mouse on the up or down arrow at the right of the field. The field scrolls in the direction of the arrows, thereby displaying previously hidden information.

At the bottom of Figure 2 are examples of several button types used in the OASIS system. Buttons connect information within the OASIS system, thereby providing links between cards. Clicking on a button takes the user to another card within the system or performs some operation on data entered in a field. In the OASIS system, there is a convention for each of the button styles used. Figure 3 shows a key for the common button symbols and icons. The check box button pictured in Figure 3 is used when a multiple choice of items in a list can be checked at the same time. The radio button shown in the figure is used when only one item in a list can be viewed at a time. The palm tree icon returns the user to the OASIS system outline.

The cards in HyperCard are in black and white. It is suggested that users with color monitors switch off the color when using OASIS because the system's visual effects will only function in black and white.

Figure 1.

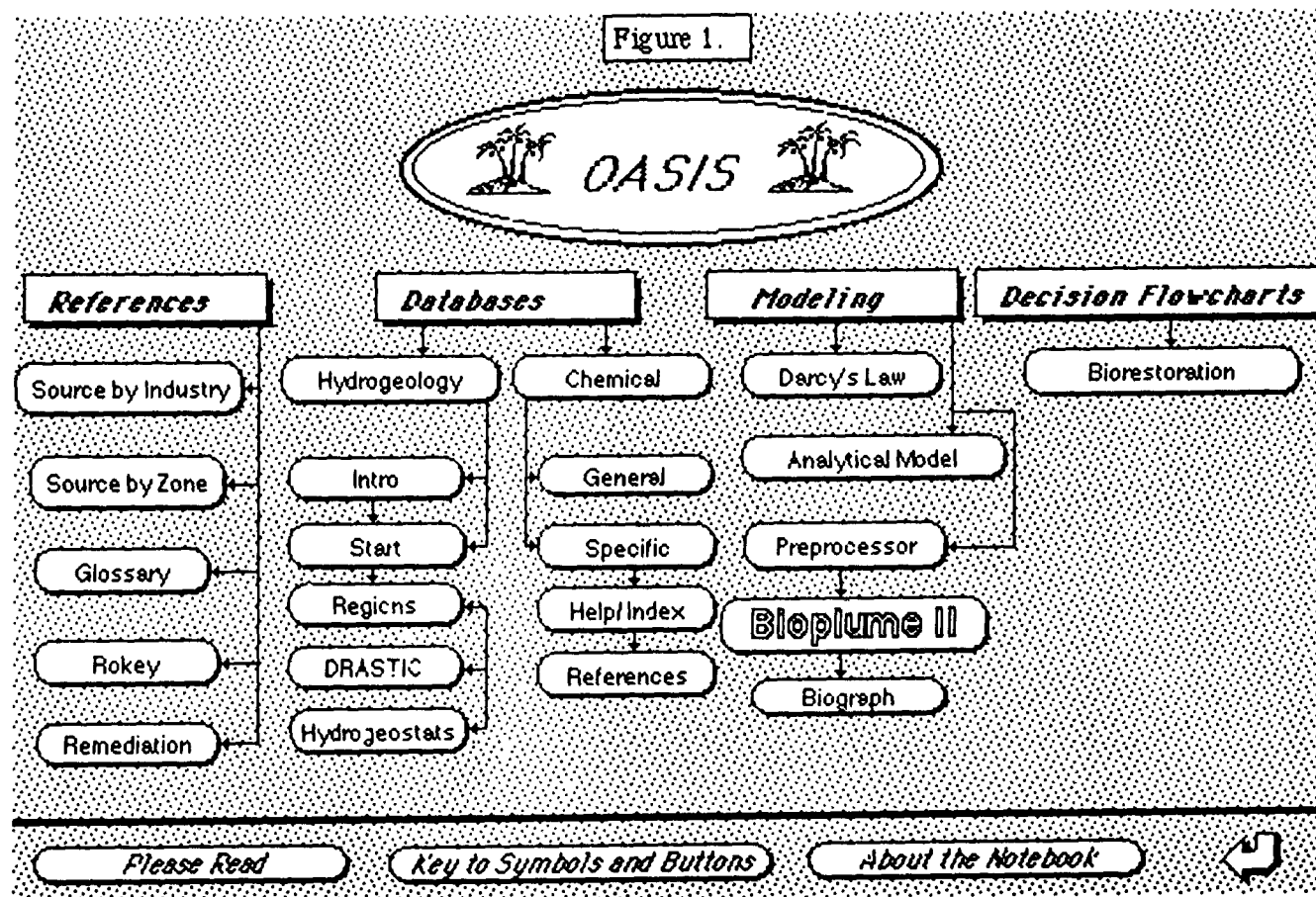


Figure 1. The system outline card for OASIS.

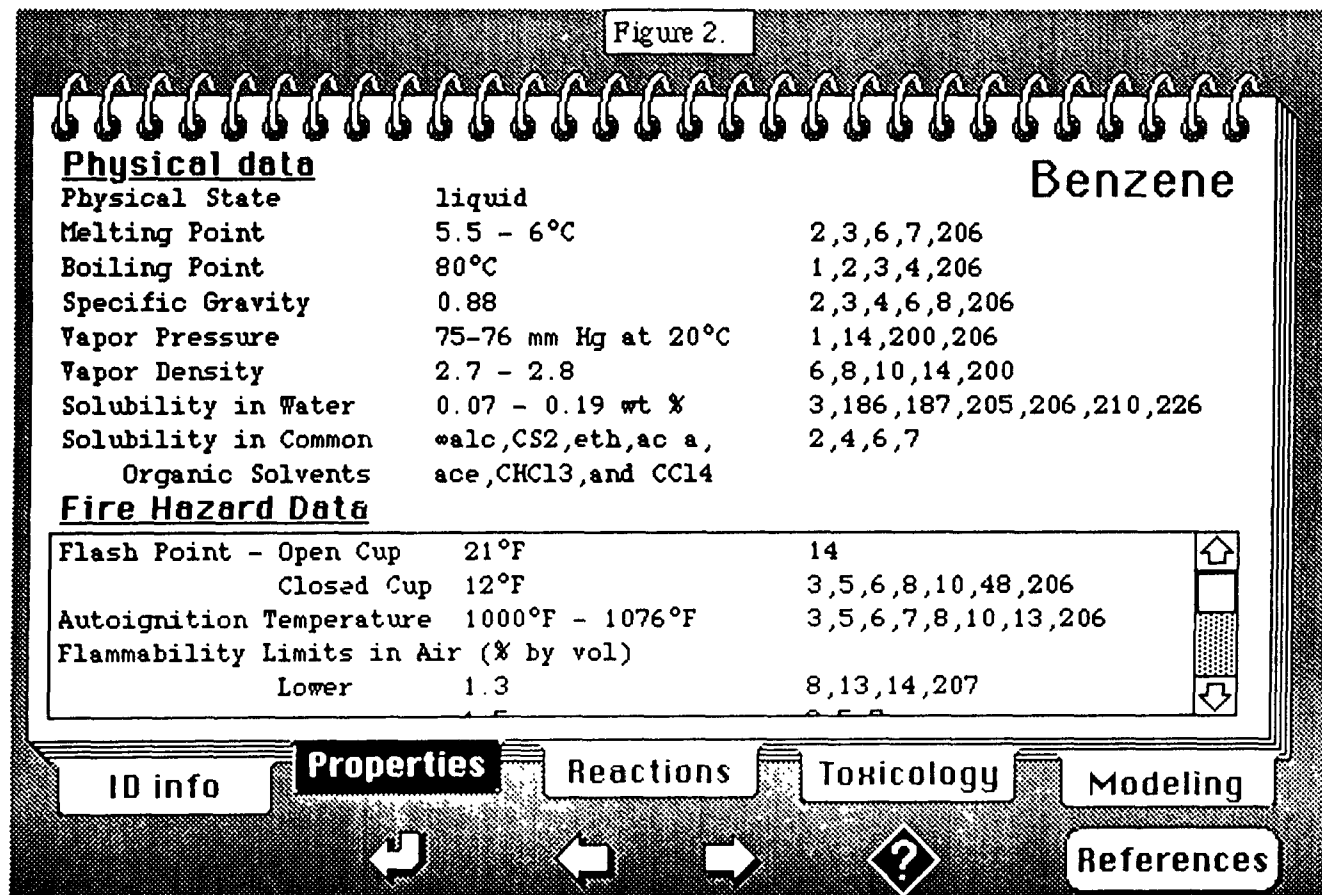


Figure 2. Card from the specific chemical database, benzene.

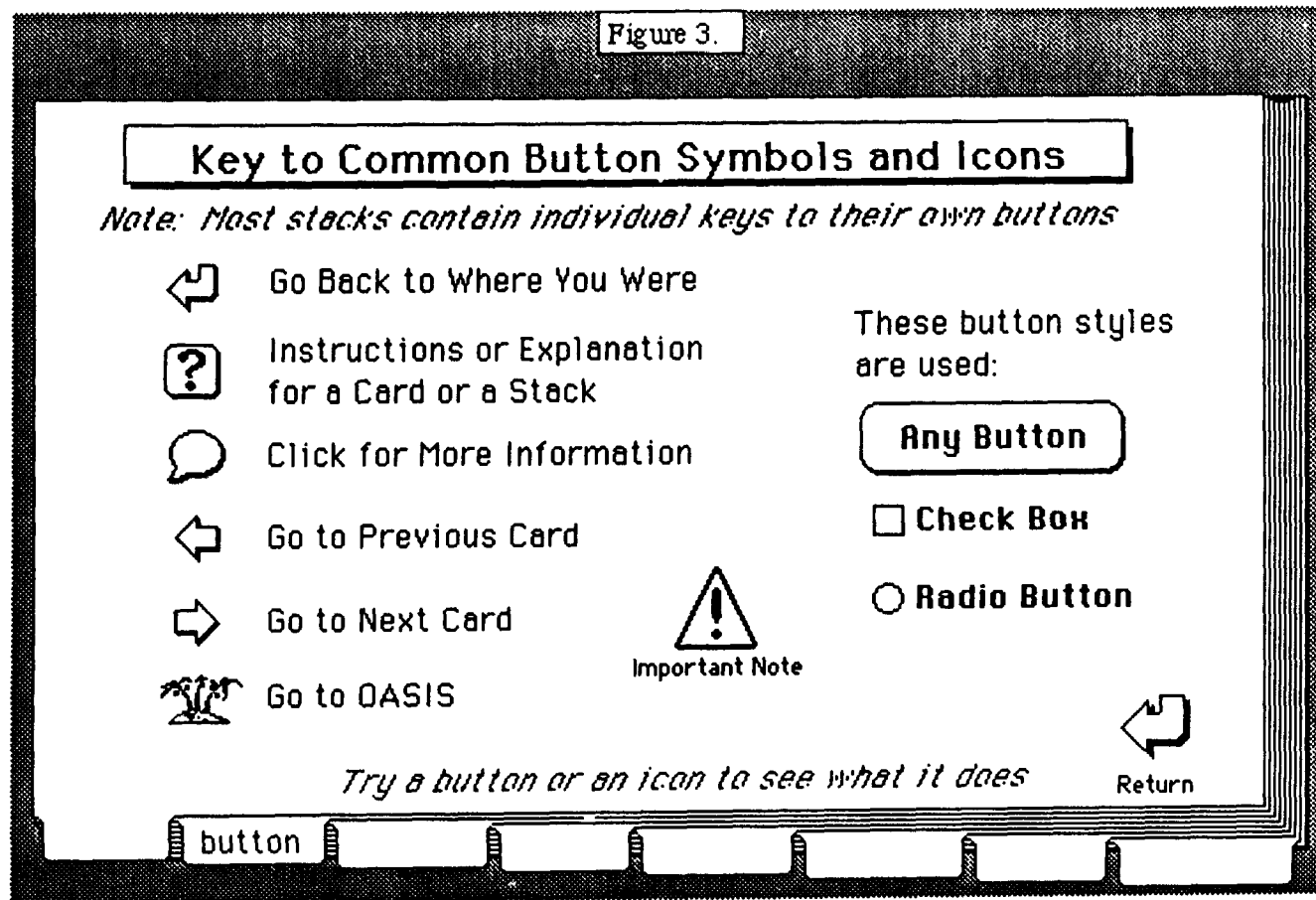


Figure 3. Key to common symbols and icons in OASIS.

Notebook

The notebook is a system within OASIS that allows the user to transfer information between stacks or from the support system to the models. For example, parameter data can be taken from the chemical or hydrogeologic stacks and put into the notebook for later use in the preprocessor. To activate the notebook, either type *Command-M* (the command key has an apple/cloverleaf on it and is located on the left-hand side of the keyboard) or use the mouse to choose the *Message* option under the *Go* menu. The message box will appear at the bottom of the screen. To operate the notebook, type one of the following three commands into the message box and hit return.

- on*** : For Open Notebook - brings up a text field into which the user may type information. The chemical and hydrogeologic databases contain a "notebook button" which, when activated, will automatically enter the relevant data from the card into the notebook.
- cn*** : For Close Notebook - hides the text field with the information saved within it. Always close the notebook before leaving a card.
- cln*** : For Clear Notebook - erases all information in the notebook.
(Note: Clear notebook only works when the notebook is closed.)
To see the whole notebook, close the message box.

WARNING: Be careful when operating the notebook. If the *cn* command is given and the notebook is not open, the notebook will be altered. If this occurs, the notebook can be repaired by clicking the *About the Notebook* button on the OASIS system outline (a routine has been placed in this button to fix the notebook if it has been altered as described).

Portions of the hydrogeologic and chemical databases also contain a button called *Notebook*. Clicking the *Notebook* button will automatically enter data from the card into the notebook and then open the notebook.

Reference Library

The reference stack contains libraries of information related to the field ground water. Figure 4 shows the flowchart for the *Source by Industry* reference stack. Clicking on any of the terms in the flowchart takes the user to contaminant information related to that source. The references stack also contains information on source by zone, a glossary of terms, the Rokey database (McClymont and Schwartz, 1987) which provides discussion of parameters used in ground water modeling, and a Remediation stack. The Remediation stack contains information on different remediation techniques for contaminated ground water aquifers and also presents BIOPLUME II simulations which demonstrate the importance of well placement and source term definition.

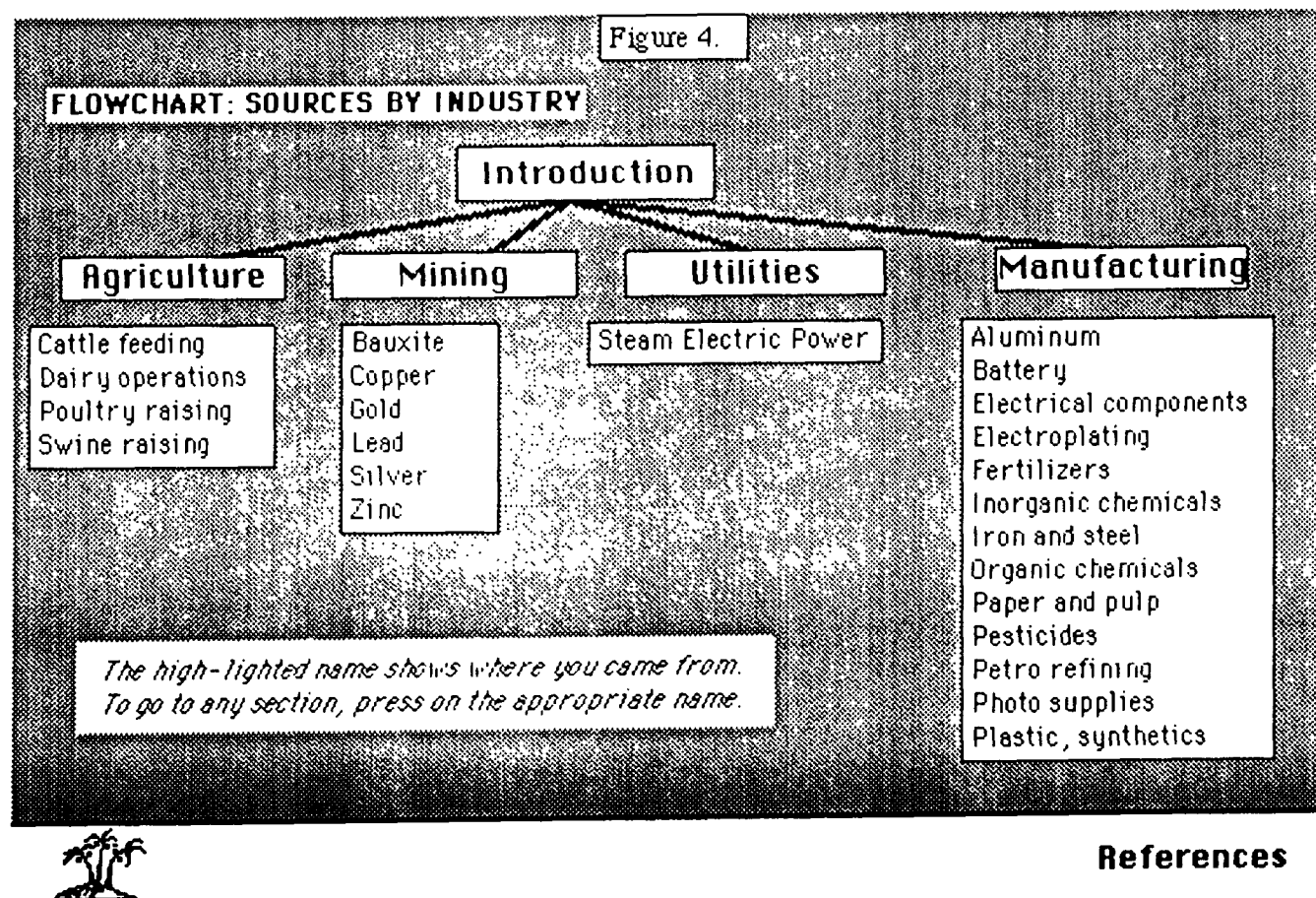


Figure 4. Flowchart from the source by industry reference stack.

Hydrogeologic Database

The hydrogeologic database was developed to take advantage of the large number of hydrogeologic investigations that have been conducted at waste sites but have not been reported in the technical literature. An extensive technical survey of ground water professionals was conducted with funding from the American Petroleum Institute and assistance from the National Water Well Association. Data from 400 field sites across the country was obtained from ground water professionals and incorporated into a database.

The database was structured using the concept of hydrogeologic settings developed for the EPA's DRASTIC system, an aquifer vulnerability index using hydrogeologic settings. The database is used by determining the hydrogeologic setting that best matches a site or area of interest. The hydrogeologic setting is selected by determining the ground water region, aquifer media, and then the setting which best describes the site in question. Figure 5 shows the decision process for selecting a hydrogeologic setting. The setting is used to access the database; the database statistics can then be used for ground water modeling or for general site characterization purposes.

After selecting the hydrogeologic setting for a site, the user is presented with two options: *Calculate DRASTIC Index* or *See Hydrogeologic Statistics*. The DRASTIC manual is presented on the *Calculate DRASTIC Index* card in the "Click for More Information" button.

The *See Hydrogeologic Statistics* option provides the mean, median, and number of cases for six parameters (hydraulic conductivity, seepage velocity, penetration depth, gradient, saturated thickness, and depth to water). The *Raw Data* and *Transformed Statistics* buttons at the bottom of the card will take the user to spreadsheets containing the data collected in the survey. Each of the six parameters exhibit a log-normal distribution, and the median values or the transformed data are probably more appropriate for most problems. The spreadsheets can be viewed using either Microsoft Excel, which does not come with the OASIS software and must be supplied by the user, or EDIT, which is supplied with OASIS. To return to the database (and HyperCard) from the spreadsheets, choose *Quit* on the pull-down menu under *File* on the menu bar. The *Hydrogeologic Statistics* section also contains a *Notebook* button which places information from the card into the notebook (for more information on the notebook see the previous discussion).

The first card in the *Hydrogeologic Statistics* section contains an *Index* button. The Index button gives the user four options: *See Data by Environment*, *See Data by Parameter*, *Collection and Analysis methods*, or *Return to Hydrogeologic DB*. The *See Data by Environment* button allows the user to view the mean, median, and number of cases for each of the six parameters once a hydrogeologic environment has been selected.

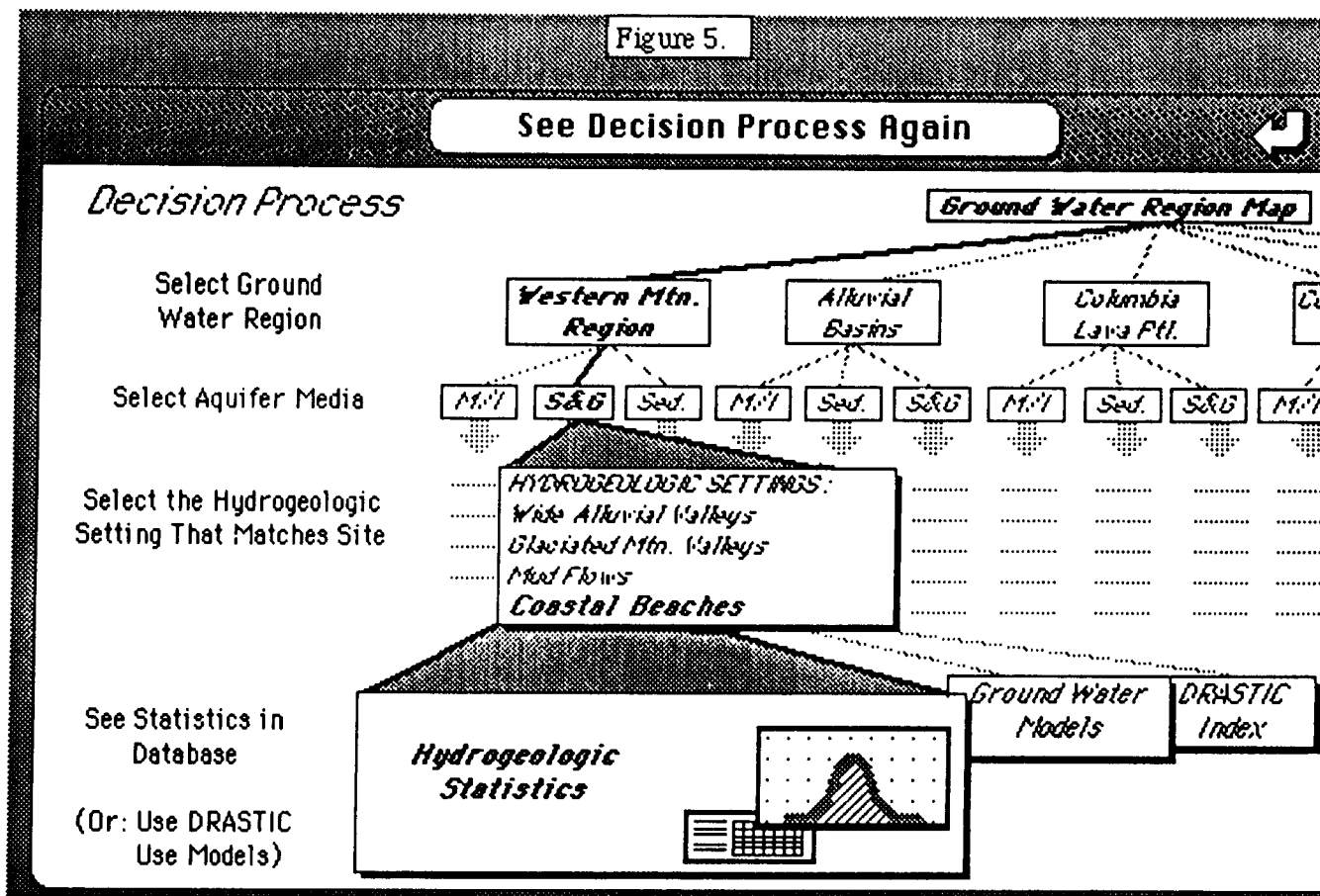


Figure 5. Decision process for selecting a hydrogeologic setting.

The *See Data by Parameter* button allows the user to select one of the six parameters and see the mean, median, and number of cases for that parameter for all the hydrogeologic environments. The *log data* and *data plot* buttons at the top of the card show the user box plots of the statistical information. If the mouse is held down on any portion of a box plot, the value at that point is displayed in a pop-up field which disappears when the mouse is released. The help button on the card explains the box plots.

The *Collection and Analysis Methods* button accesses "Hydrogeologic Database for Ground Water Modeling" (Newell, Hopkins, and Bedient, 1988), a report which discusses the database in more detail. The *Return to Hydrogeologic DB* option returns the user to the *Calculate Drastic Index/See Hydrogeologic Statistics* card.

General Chemical Database

The general chemical database contains 117 chemicals with one card of information per chemical and was taken from the ROKEY database by McClymont and Schwartz, 1987 (original source: Federal Register, 1982). Chemical information can be accessed in four ways: by category, by name, by EPA number, or by CAS number (Chemical Abstract Service number). The general chemical database contains a *Notebook* button which enters data from the card into the notebook (for more information on the notebook see the previous discussion). Figure 6 shows the benzene card from the database.

Specific Chemical Database

The specific chemical database contains 18 chemicals with 25 cards of information per chemical. The first card of the database has buttons which access information related to *Identification*, *Physical Properties*, *Fire Hazard Data*, *Chemical Reactions*, and *Toxicology*. These terms are defined as they are used to describe the various chemicals in the database

The *Choose Chemical* button allows the user to select, by name, a chemical from the database. Figure 2 shows a card from the specific chemical database for benzene. The physical and fire hazard data are given. A list of numbers is shown to the right of the data. These numbers are the reference numbers related to each piece of information. Clicking on a number will take the user to that reference in the reference list. Please note, however, that words and phrases which are not reference numbers can also be chosen with the mouse for the reference search. Should this happen, an appropriate error message will occur.

The first card of the specific chemical database also contains a button named *Find a Phrase*. This button will search the stack and take the user to the first card in which the phrase is referenced. Hitting return after a reference is found will continue the search procedure.

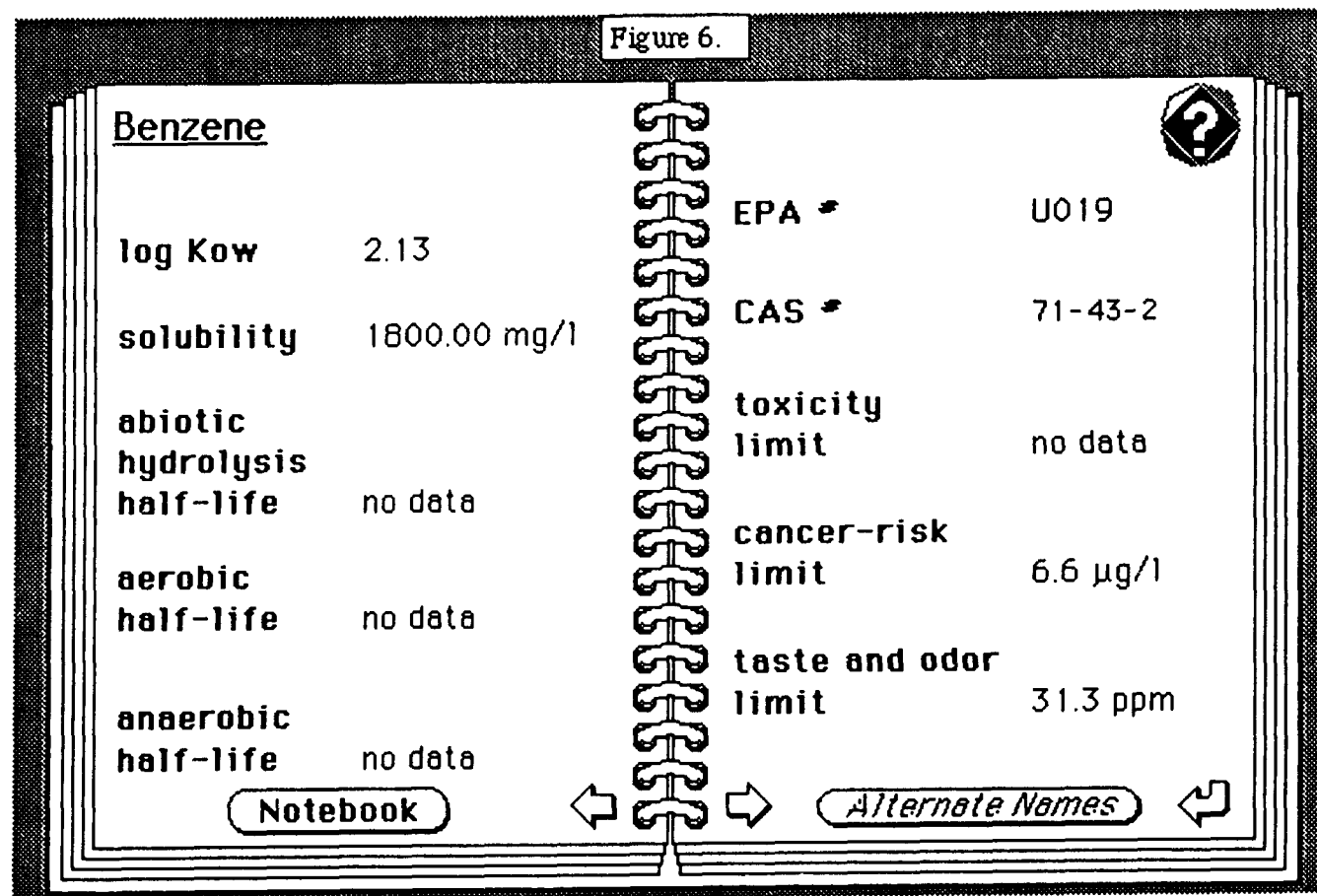


Figure 6. Card from the general chemical database, benzene.

Darcy's Law

The Darcy's law stack calculates the ground water velocity in a system where hydraulic conductivity, gradient, and porosity are known. The help button (question mark icon) gives information for each of the parameters needed in the calculation.

Analytical Models

Currently, only one analytical model is contained in this stack. ODAST (Javandel, Doughty, and Tsang, 1984) is a one-dimensional solute transport model, which considers advection, dispersion, solute decay, source decay, and adsorption. Output from the model is provided as a two-way table of dimensionless concentration versus time and distance. The ODAST model is a useful tool for providing preliminary estimates of solute transport in a ground water system.

To run ODAST, the user first enters data into the ODAST data input card. The help button (question mark icon) contains definitions for the input variables, as well as the equations used by ODAST. After entering the data, the user must save the data to an input file. After hitting the "Save" button, a standard save-file dialog box will appear onscreen. This box allows the user to decide where to save the input file on the hard disk. ODAST input data sets must be in the Analytical Models folder to be accessed by the program. The system will also prompt the user to enter a title for the file being saved to disk. The "Run ODAST" button will open the program. The user will be prompted to enter an input data set name and an output data set name. The "View Data" button on the ODAST input data card opens the Edit application, and allows the user to see the input or output file for an ODAST run. The help button on the input data card also explains the procedure for running ODAST.

BIOPLUME II Model

BIOPLUME II is a two-dimensional computer model that simulates the transport of dissolved hydrocarbons under the influence of oxygen-limited biodegradation. BIOPLUME II also simulates reaeration and anaerobic biodegradation as a first order decay in hydrocarbon concentrations. The model is based on the USGS solute transport two-dimensional code (Konikow and Bredehoeft, 1978). BIOPLUME II computes the changes in concentration over time due to advection, dispersion, mixing, and biodegradation.

BIOPLUME II solves the solute transport equation twice: once for hydrocarbon and once for oxygen. As a result, two plumes are computed at every time step. The model assumes an instantaneous reaction between oxygen and hydrocarbon to simulate biodegradation processes. The two plumes are combined using the principle of superposition.

The model is extremely versatile in that it can be used to simulate natural biodegradation processes, retarded plumes, and in-situ bioremediation schemes. BIOPLUME II allows injection wells to be specified as oxygen sources into a contaminated aquifer, and the model can be used to evaluate alternate methods for aquifer reclamation.

BIOPLUME II PreProcessor

A graphical preprocessor for the BIOPLUME II model has been developed to facilitate data entry. Figure 7 shows the first card of the BIOPLUME II PreProcessor. This card is divided into three sections, from left to right across the screen. These sections are Start Here, Enter Data for Model, and Run Model.

Start Here

The Start Here section contains two buttons: Clear PreProcessor and Import existing file.

Clear PreProcessor. HyperCard automatically saves changes made to the preprocessor. Any previous work which has been done and not cleared will be stored in the preprocessor. Therefore, to begin a completely new data set, the user must use the *Clear PreProcessor* button. Otherwise, the existing preprocessor file may be edited.

Import a File. The *Import a File* button imports to the preprocessor a data set which has been saved previously. **Warning:** Importing a file is a slow process (up to 35 minutes for a Mac SE), and it may be faster to re-enter the data by hand.

Enter Data for Model

Data is entered in six sections: *Configuration, Timing Parameters, Physical Parameters, Initial Conditions, Boundary Conditions, and Numerical Parameters*. **Note:** Data must be entered in decimal format; exponential notation cannot be read by the preprocessor.

The first card of the preprocessor contains a "New Users Click Here!" button (question mark icon). This button contains important information for running the BIOPLUME II model. This button contains a Read This First section, a BIOPLUME II summary, BIOPLUME II assumptions, a Troubleshooting section (i.e., what to do about long run times and high mass balance errors, and the run time error codes for the model), a Guided Tour of the Array Maker, and a Disclaimer for BIOPLUME II. Every user is strongly urged to read through the new user's information. Also, the BIOPLUME II user's manual can be accessed from the first card of the preprocessor ("*BIOPLUME II Manual*" button).

The Configuration card must be completed before data is entered on any other card. The Configuration card defines the model grid to be used in the simulation. When each data section is complete, the corresponding button on the first card of the preprocessor will be highlighted, as seen in Figure 7. All six data sections must be completed before the preprocessor file is *Saved to Disk* and used as an input data set for the model. Also, the user must enter data for every variable in the preprocessor. If the value for a variable is left blank, a run time error will result.

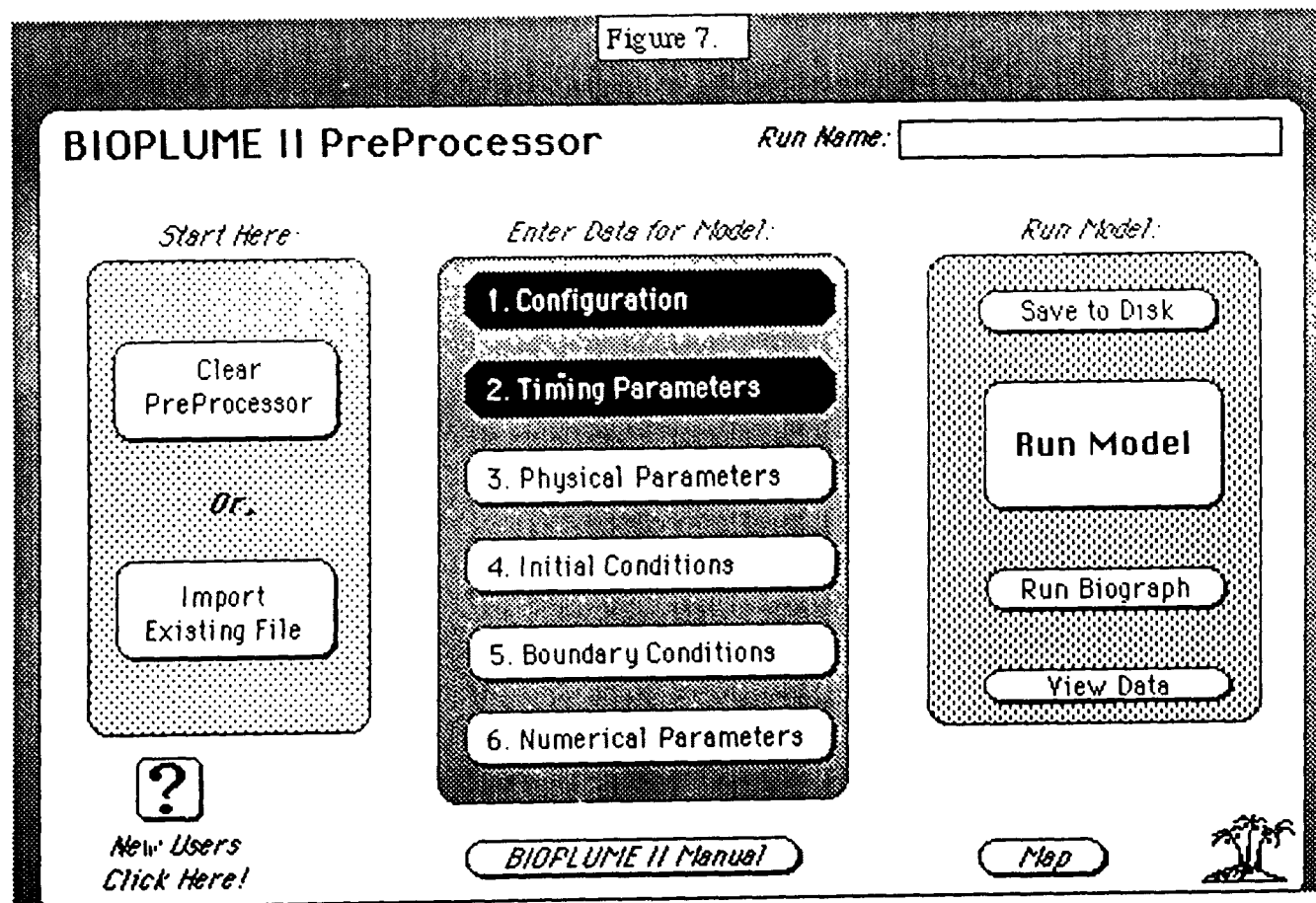


Figure 7. First card from the BIOPLUME II preprocessor.

All cards in the preprocessor contain help buttons (question mark icon), which assist the user in completing the data set. Help buttons next to the parameter will give a definition and typical values for a given parameter. The user is strongly urged to use the help buttons whenever she or he has questions.

Using the Array Maker. Certain parameters in the model require that a value be entered for every grid cell. A 10 x 10 grid, for example, would require 100 values to be entered for the parameter; the group of data values is referred to as an array. An array may have a different value for every grid cell, blocks of areas with the same value, or a constant value over the entire grid. Entering a large number of values into an array can be tedious. However, the BIOPLUME II PreProcessor has an easy, graphical approach for entering data into arrays (the array maker), which helps facilitate the process.

Figure 8 shows the transmissivity card from the preprocessor. A 20 x 20 grid is shown, with different patterns displayed over the grid. Each pattern corresponds to a different value of transmissivity. The key to the transmissivity values is shown to the right of the grid. To use the array maker, the user first selects a value for transmissivity (see the white arrow pointing at a value of 0.001 ft²/s in Figure 8). The mouse is then clicked at the upper left-hand corner of the area which will be described by the selected value of transmissivity. Without releasing, the user drags the mouse to the lower right-hand corner of the area. A flashing rectangle will show the chosen area (see Figure 8). When the mouse is released, the appropriate pattern will fill the area. The patterns on the grid are automatically converted into a numerical array.

Important: Simply clicking on a value in the grid key will not enter data into the numerical array, which is used in the BIOPLUME II model. The user must go through the click and drag procedure. Similarly, if any changes are made to the grid key values, the user must click and drag after the changes have been made, or the numerical array will not reflect the changes. Also, if the number entered for a variable is not on the list of pattern values, the default pattern will be black. Black patterns may occur when importing a file, if the user manually changes values in the list of pattern values, or if the user enters data with the *Other Data Entry Options* button (below), and the values entered do not correspond to the pattern values. To change black patterns, the user needs to change the values in the pattern list to correspond to the values entered for the variable. Then the click and drag procedure must be performed before the grid patterns will change. See the Troubleshooting section (accessed through the help button on the first page of the preprocessor) for more information.

The numerical array can be seen at any time by clicking the *Other Data Entry Options* button on the card (see Figure 8). This button not only allows the user to view the array, but also allows him/her to enter data in one of two ways: as a constant value over the entire grid by typing a single number or as discrete values, entered one at a time, directly into the array.

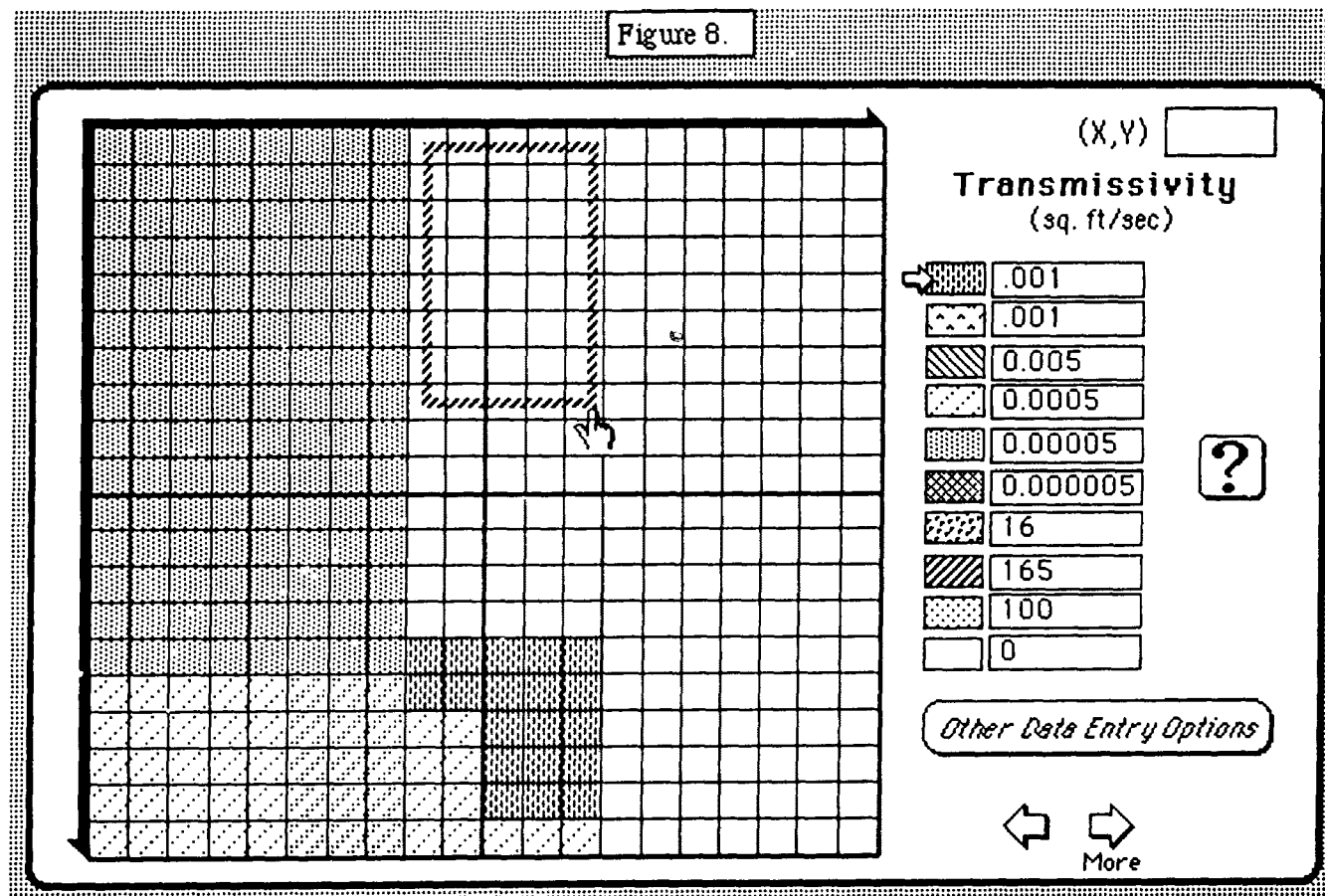


Figure 8. Transmissivity card.

The help button (question mark icon, see Figure 8) gives information about transmissivity and also shows a guided tour of the array maker. On the first card of the preprocessor, also, there is a *New Users Click Here!* button, which contains the guided tour of the array maker. It is strongly urged that first time users watch the guided tour before entering data into the array cards.

The following parameters require that data be entered as a numerical array:

Physical Parameters

- Transmissivity
- Saturated thickness
- Diffuse recharge

Initial Conditions

- Initial water table
- Initial contaminant concentration
- Initial oxygen concentration (only if aerobic degradation)

Boundary Conditions

- Constant head cells
- Area sources

The default value for parameters entered as an array is zero, (i.e., a value of zero is entered into the arrays until the user makes changes). For all non-array variables, the user must enter a value; there is no assumed default.

Run Model

The Run Model section contains four buttons: *Save to Disk*, *Run Model*, *Run Biograph*, and, *View Data*.

Save to Disk. The *Save to Disk* button saves the current preprocessor file in a format which can be used by the BIOPLUME II model as an input data set. The user must *Save to Disk* before using a preprocessor file to run the model. After hitting the "Save to Disk" button, a standard save-file dialog box will appear onscreen. This box allows the user to decide where to save the input file on the hard disk. The best place to save the input file is in the BIOPLUME II folder. If the user opens the BIOPLUME II folder in the minifinder (save file dialog box) before hitting the save button, the file will be saved in that folder.

Run the Model. The *Run Model* button accesses BIOPLUME II. The user needs to supply an input file name (created by *Saving to Disk*). The user will then be prompted for names for an output file and for a BioGraph file (the default name for the postprocessor file will be "input file name Biograph" file). The BioGraph file created during the BIOPLUME II run is used as input for the postprocessor. To return to HyperCard when the run is finished, the user simply needs to hit the carriage return on the keyboard.

A BIOPLUME II run can take anywhere from a few minutes to a few hours. To estimate the time required to complete a BIOPLUME run, see the "Long Run Times" in the Troubleshooting section (accessed by clicking on the help button on the first card of the preprocessor). To cancel a run before completion, type command (the apple/cloverleaf key) and a period at the same time.

Run BioGraph. The *Run BioGraph* button accesses BioGraph, a graphical post-processor for the BIOPLUME II model. The input for BioGraph is the BioGraph file created during the model run. To return to HyperCard when finished in the postprocessor, the user must choose *Quit* on the pull-down menu under *File* on the menu bar. For more information on BioGraph, see the BioGraph user's manual in Section 9.0.

View Data. The *View Data* button takes the user to the Edit application. Edit allows the user to see the data set which will be used as input for BIOPLUME II. Edit also will allow the user to view the output data set created by BIOPLUME II. To use the *View Data* button, the user needs to click the button and supply a file name. To return to the preprocessor when finished, the user must choose *Quit* on the pull-down menu under *File* on the menu bar. **Note:** The data must be saved (using the *Save to Disk* button) before the *View Data* button can be used to view the input data set.

OASIS Example

As an example of the way in which OASIS can be used as a support tool for the BIOPLUME II model, consider a gasoline leak at a service station located in the western mountain ranges. The following steps might occur when using the system.

First, the user might consult one of the two chemical databases contained in OASIS. The user could refer to the specific chemical database to examine physical data on benzene (Figure 2).

If the user is unfamiliar with the hydrogeology of the area, he or she can enter the hydrogeologic database. The correct ground water region is selected first, then the aquifer media, and then the hydrogeologic setting, as pictured in Figure 9. Once the setting is known, the user can examine data from sites with a similar hydrogeologic setting. The hydrogeologic data is designed to be used as a general educational tool and is not designed to be a substitute for field work.

At this point, the user can run the analytical model to help set up the problem or enter directly into the BIOPLUME II PreProcessor. The preprocessor was designed to do three things: structure the data entry process, give immediate access to ground water and data entry help, and provide a graphical method for entering and viewing the spatial information used by the model.

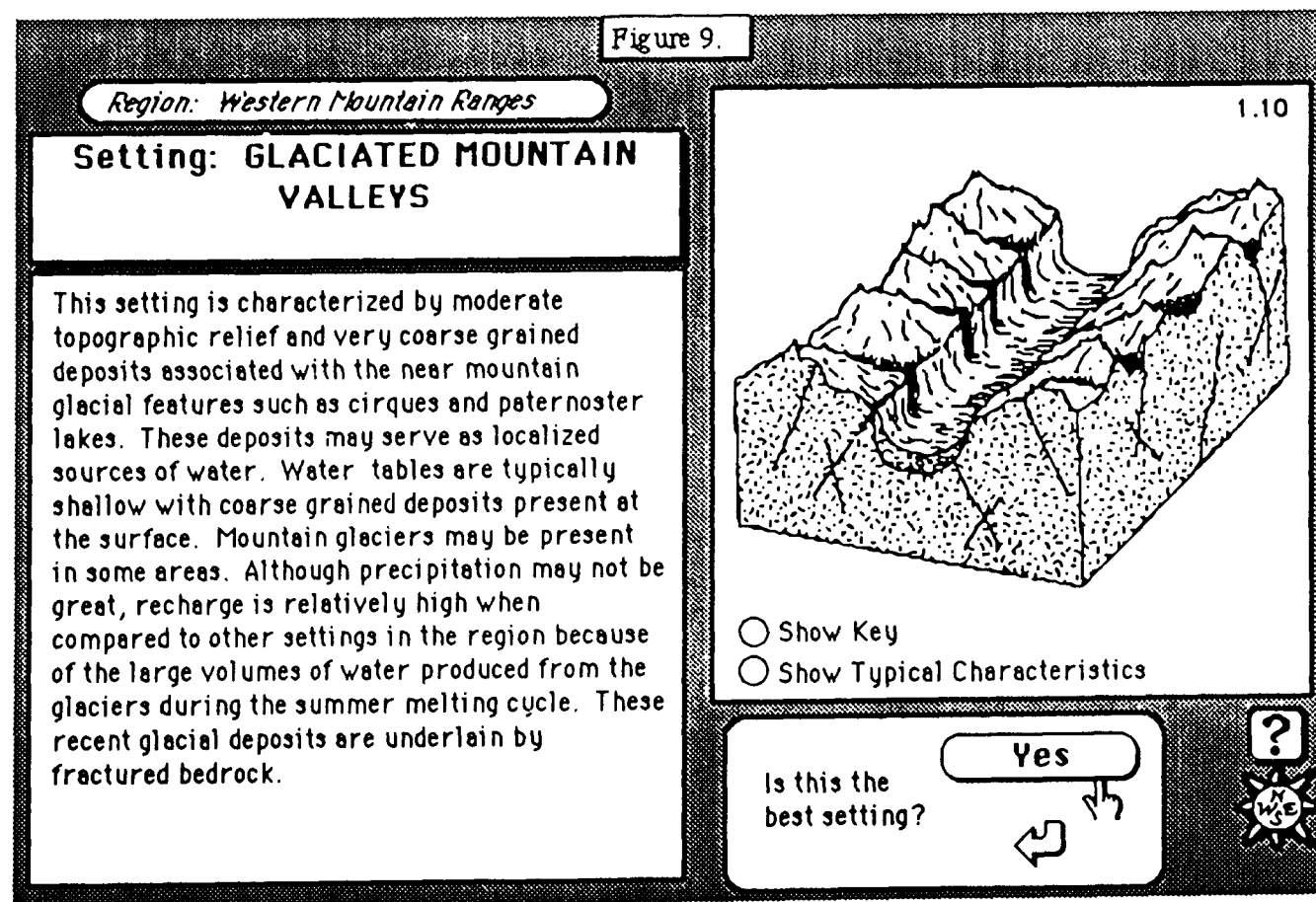


Figure 9. Hydrogeologic setting card.

Once the user finishes entering the data, the preprocessor makes a text file corresponding to the format required by BIOPLUME II. The model is run and the graphical postprocessor, BioGraph, displays the output from the model (contaminant concentrations over the area of the aquifer) in the form of patterns. Darker patterns correspond to higher concentrations. The development of the plume over time can be seen with an animation option in BioGraph. Concentration profiles over time or over distance (Figure 10) can be examined also. The preprocessor and the postprocessor for BIOPLUME II were designed to facilitate model calibration and data evaluation.

File Modes Time Windows Other Info Color
Hydrocarbon Plume

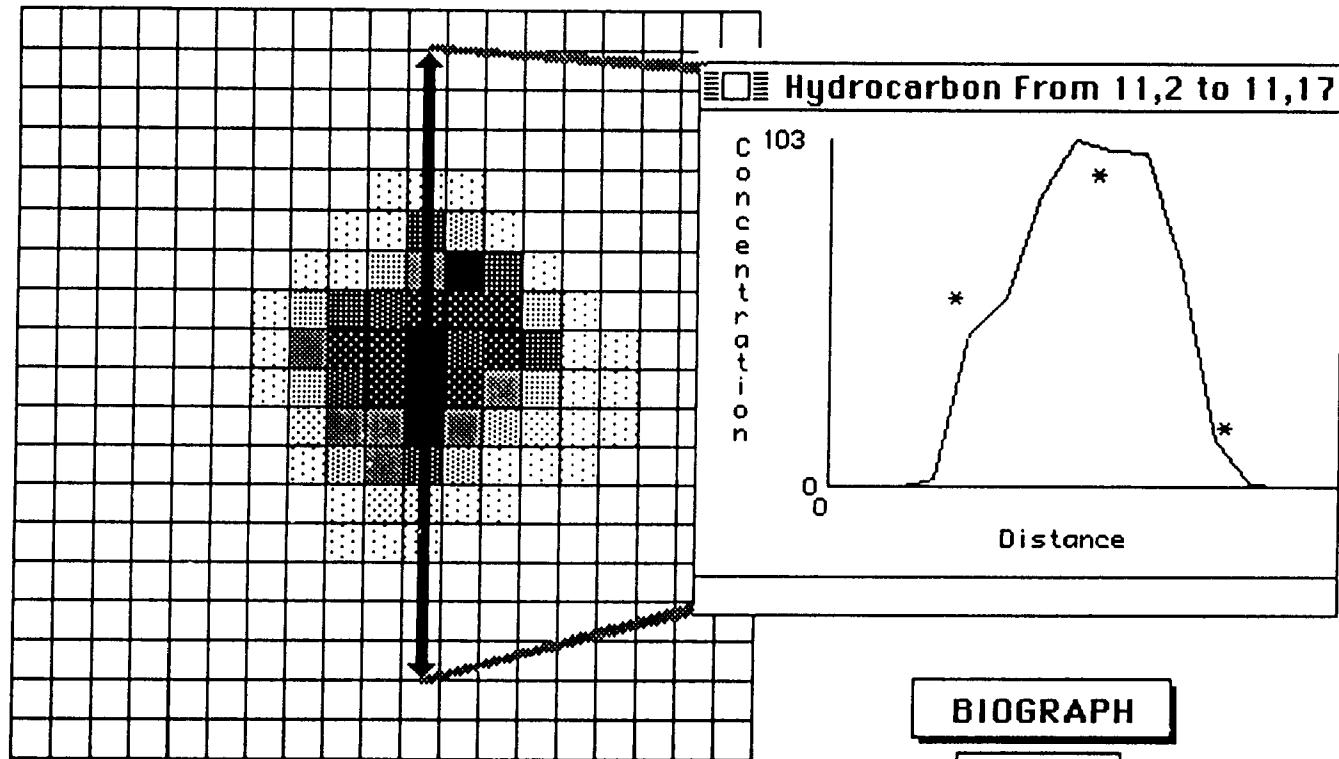


Figure 10. Output from the BioGraph postprocessor.

4.0 OASIS SYSTEM REQUIREMENTS

The OASIS system will run on an Apple Macintosh SE, Macintosh II, IIx, IICx, or SE/30 computer. The system requires 9 Mb of hard disk storage and **1 Mb of RAM**. If your computer has insufficient internal memory to run OASIS, the BIOPLUME II PreProcessor will not run properly. Indications of memory problems include the following:

- Dialog boxes which inform you that there is not enough memory to use the paint tools
- Dialog boxes which inform you that a picture cannot be saved

If your computer experiences memory problems while running OASIS, make sure that your computer's RAM cache is turned off. To check the RAM cache, look in the Control Panel which is located in the pull-down menu under the apple on the menu bar. Also, no networking software or applications such as multifinder should be in operation.


The Macintosh SE may not be suitable for running BIOPLUME II for many problems due to the lack of a math co-processor in the SE. Problems involving high ground water velocities, large grid sizes, pumping wells, or injection wells may require excessive run times on a Mac SE. See the Troubleshooting section (accessed through the help button on the first card of the preprocessor) for information on:

- How to estimate run times
- How to cancel runs
- How to speed up runs

The Macintosh II, IIx, IICx, and SE/30 are much faster at performing heavy numerical calculations and can handle more numerically intensive simulations.

5.0 INSTRUCTIONS FOR INSTALLING THE OASIS SOFTWARE

These instructions are fairly comprehensive and will ensure proper operation of the OASIS system on your computer. Please follow them closely and make sure you complete each step. Do not hesitate to call for assistance if you have any questions or problems (Rice University, Department of Environmental Science and Engineering, (713) 527-4951). If at any time during the installation you encounter a situation not covered in these instructions, please note the circumstances and call for assistance. If the system is not properly installed, you may encounter problems with its operation. If you accidentally throw a file or stack away, you may have to re-install the whole system. If you are an experienced Macintosh user, an abbreviated version of the installation procedures follows this section.

1. **Remove ALL old OASIS files** from your hard disk. If you are unsure if some files are part of the old OASIS system, please make a list of them and call us.
2. Move to the desktop level and note the name of your hard disk. The desktop is explained in the Macintosh user's manuals. The easiest way to move to the desktop is to hold down the option key and click in the close box in the upper left-hand corner of the front-most window. This will close all open windows. You should see a trash can icon and the hard disk icon. Make a note of the hard disk name, which appears at the bottom of the disk icon. Be sure to include any spaces or other special characters, as they are important. Now double-click the hard disk icon to open it. The window which appears is called the desktop window.
3. Make sure there is no folder on the desktop called "OASIS Folder" or "Temporary OASIS Folder." If there is, either throw it away (if it contains nothing you want to keep) or rename it to something else. **Also make sure that Multifinder is turned off when loading OASIS.** If Multifinder is on or you are unsure, choose the Restart command from the Special menu while holding down the command key (the command key has the  icon on it). Hold down the command key until the computer has completely finished rebooting.
4. Check to see that there are at least 10 Mb free on your hard disk. You must have at least 10 Mb to use the system. The free space is shown in the upper right of the window, just below the title. 10 Mb is equal to 10240 K. If there is not enough space, you will have to remove other items. If this is the case, when you have cleared at least 10 Mb on your disk, please return to the desktop level (as described in step 2) and continue with the installation.
5. Find the HD Backup application that came with your Macintosh computer. If it is already on your hard disk, skip to step 7. If not, continue with step 6.
6. HD Backup can be found on the Utilities disk or disks that come with every Macintosh computer. Insert these disks until you find one with the application HD Backup, then copy it to your hard drive by clicking on its icon and dragging it onto the desktop window of your hard disk.
7. Double-click the application icon named "HD Backup." This will start the HD Backup application.

8. Click the button labeled "Restore a single file.", then click the button labeled "OK."
9. Insert the first disk, labeled "OASIS Part 1 - Disk 1". The file "1.OASIS Part 1 (Compressed)" should be highlighted (if not, click on that file name). Click "Open."
10. Insert each of the Part 1 disks as they are requested from 2 through 6.
11. When the restoration is completed, click on the button "Quit." The application may ask for the last disk inserted. If so, insert the disk OASIS Part 1 - Disk 6 as directed.
12. At the desktop level, there will be a compressed file on your hard drive called "OASIS Part 1 (Compressed)". Open it by double-clicking on it. The computer will proceed to decompress the file. This takes approximately 20 minutes on a Macintosh SE.
13. There will now be a folder on the hard drive called "OASIS Folder" in addition to the file "OASIS Part 1 (Compressed)." Put "OASIS Part 1 (Compressed)" in the trash can by clicking its icon and dragging it over the trash can on the lower-right side of the screen. Click on the menu button Special at the top of the screen, drag down to the command "Empty Trash," and release the mouse button. From now on in the instructions, when a menu and a command are given, do them in this manner.
14. Double-click the application icon named "HD Backup." This will start the HD Backup application again.
15. Click the button labeled "Restore a single file.", then click the button labeled "OK."
16. Insert the first disk, labeled "OASIS Part 2 - Disk 1." The file "1.OASIS Part 2 (Compressed)" should be highlighted (if not, click on that file name). Click "Open."
17. When requested, enter the disk labeled "OASIS Part 2 - Disk 2."
18. When the restore is completed, click on the button "Quit." The application may ask for the last disk inserted. If so, insert the disk OASIS Part 2 - Disk 2 as directed.
19. There are now two OASIS icons on your hard disk, "OASIS Folder" and "OASIS Part 2 (Compressed)." Open "OASIS Part 2 (Compressed)" by double-clicking on it. The computer will proceed to decompress the file. This takes approximately six minutes on a Macintosh SE.
20. There will now be a folder on the hard drive called "Temporary OASIS Folder" in addition to the file "OASIS Part 2 (Compressed)" and "OASIS Folder." Put "OASIS Part 2 (Compressed)" in the trash can by clicking its icon and dragging it over the trash can on the lower-right side of the screen. Do the "Empty Trash" command from the Special menu.
21. Open the Temporary OASIS Folder by double-clicking on it. Make sure the window showing the files in the Temporary OASIS Folder does not cover the icon of the OASIS Folder. If it does, resize or move the Temporary OASIS Folder window until it does not. Choose the "By Kind" command from the View menu. Choose the "Select All" command from the Edit menu. Put all of the files in the Temporary OASIS Folder into the OASIS Folder by clicking on any of the small, darkened icons in the Temporary OASIS Folder window, drag them over the OASIS Folder icon until it is darkened, and then release the mouse button, dropping the files into the OASIS Folder.
22. Close the Temporary OASIS Folder window by clicking on the small square in the upper-left corner of the window.

23. Throw away the Temporary OASIS Folder by dragging it into the trash can and choosing the "Empty Trash" command from the Special menu.
24. Open the OASIS Folder by double-clicking on its icon. Choose the "By Kind" command from the View menu.
25. The OASIS folder contains your OASIS software. **Please do not move this folder, rename it, or otherwise change the file structure. Please do not change the names or locations of any of the files inside the folder,** except input and output files for the BIOPLUME and BioGraph programs.
26. You will see one icon, named "HyperCardv1.2.2.," at the top of the list. Double click this icon to start the OASIS system. Even if you do not wish to use the software at this point, you must start it up in order to initialize the file structures.
27. Click on the button labeled "Read This First." Then click "Update Hard Disk Name."
28. You will be asked if you know the name of your hard disk. If you wrote the name down in step 2, click yes. Otherwise click Help and follow the instructions on how to get the name of your hard disk. When you do know the name, return to this step.
29. In the next dialog box, type in the name of your hard disk, including any spaces, etc., then click OK.
30. **Use the "Update Hard Disk Name" button anytime you change the name of your hard disk.** You may now click on the OASIS button to enter the system or use the "Quit" button to quit HyperCard.

Note: You may keep HyperCard on your hard disk for other uses, but you must use a separate copy of the program file, and that copy must be in a different folder. None of the OASIS files can be merged into other HyperCard environments at this point. **Do not leave any of your own HyperCard stacks in the OASIS folder.**

6.0 OASIS INSTALLATION PROCEDURE FOR EXPERIENCED USERS

This installation procedure is for users who are already familiar with the Macintosh environment. If you are unsure or have questions about any part of this procedure, use the more detailed instructions in the user's manual. First, make sure that your hard drive meets these four conditions:

1. Does not contain any old OASIS files.
2. Does not have a folder called "OASIS Folder" or "Temporary OASIS Folder."
3. Has at least 10 Mb of free disk space.
4. Multifinder is turned off (do this temporarily by restarting the Mac with the command key down).

Procedure

1. Find the copy of the program HD Backup which comes with every Macintosh computer on the Utilities disk(s). Put it on your hard drive if it is not there already.
2. Run the HD Backup application.
3. Click "Restore a single file." and "OK."
4. Insert the first disk, labeled "OASIS Part 1 - Disk 1". Open the file "1.OASIS Part 1 Compressed)."
5. Insert each of the Part 1 disks as they are requested from 2 through 6.
6. Quit the HD Backup application.
7. There will be a compressed file on your hard drive called OASIS Part 1 (Compressed). Open it. The computer will proceed to decompress the file. This takes approximately 20 minutes on a Macintosh SE.
8. There will now be a folder on the hard drive called OASIS Folder in addition to the file OASIS Part 1 (Compressed). Put OASIS Part 1 (Compressed) in the trash can and do the Empty Trash command from the Special menu.
9. Run the HD Backup application again.
10. Click "Restore a single file." and "OK."
11. Insert the disk labeled "OASIS Part 2 - Disk 1." Open the file "1.OASIS Part 2 (Compressed)."
12. Insert the disk labeled "OASIS Part 2 - Disk 2" when requested.
13. Quit the HD Backup application.

14. There will be a compressed file on your hard drive called OASIS Part 2 (Compressed). Open it. The computer will proceed to decompress the file. This will take approximately six minutes on a Macintosh SE.
15. There will now be a folder on the hard drive called Temporary OASIS Folder in addition to the file OASIS Part 2 (Compressed). Put OASIS Part 2 (Compressed) in the trash can and do the Empty Trash command from the Special menu.
16. Open the Temporary OASIS Folder, choose "By Kind" from the View menu, choose the "Select All" command from the Edit menu, and drag all four files at once from the Temporary OASIS Folder and drop them into the OASIS Folder.
17. Put Temporary OASIS Folder in the trash can and do the Empty Trash command from the Special menu.
18. Open the OASIS Folder and select the "By Kind" command from the View menu. At the top of the list should be Hypercardv1.2.2. Opening this will start OASIS.
19. Run HyperCardv1.2.2 inside the OASIS Folder and follow the instructions given by the "Read This First" button.

Note: Never change the name of the OASIS Folder and never change the name or location of any of the items inside the folder, except for input and output files that you make yourself.

7.0 USING OASIS

Whenever you wish to use the OASIS software, use the following simple procedure to enter the system:

1. Close all open windows. You can do this easily by holding down the option key and closing the front-most window. All other windows will automatically close.
2. Open the hard disk icon - this will get you to the desktop window.
3. Open the folder named "OASIS Folder."
4. Double-click the HyperCardv1.2.2 icon which will appear in the OASIS Folder window.
5. If you have changed the name of your hard disk, use the button labeled "Update Hard Disk Name."
6. Click the button labeled "OASIS" to enter the system.

If you encounter any problems while using the software, please refer first to the Macintosh user's manual. Many "problems" are actually just standard operating system procedures. If you seem to be getting a lot of standard file dialog boxes asking "Where is ...," you may need to update the name of your hard disk, as described above. If you need to leave the system at any time or the system appears to be "hung," you can exit by holding down the command (apple/cloverleaf) key and typing a "q." This will return you to the desktop level. If this does not work, try holding down the command key and typing a period (.). If all else fails, simply turn off the computer. You can re-enter the system after you restart the machine. If you ever become lost in the system, the OASIS palm tree icon will return you to the system outline. Also, selecting "Home" on the pull-down menu under "Go" on the menu bar will take you to the OASIS Home card.

8.0 GENERAL OASIS EXERCISES

The following questions and exercises are intended to help you navigate through the OASIS system. Begin at the system outline. The italicized words in the answers show the sequence of button selections needed to arrive at the correct information. The first word preceding the italicized button selections is the stack name.

Reference Library

1. Question: What is the difference between 'Total porosity' and 'Effective porosity'?

Answer: *References, Rokey, Porosity.*

- Total porosity = total void space in porous material
- Effective porosity = that portion of total porosity which is interconnected

Chemical Database

2. Question: What are two other names for the eighth monocyclic aromatic compound listed? What is its toxicity limit?

Answer: *Databases, Chemical, General Chemical Database, Category, Monocyclic aromatic.* Go to the eighth chemical.

- Phenylethane, ethylbenzol
- 1400 mg/l

3. Question: What is the aerobic half-life of naphthalene?

Answer: *Databases, Chemical, General Chemical Database, Name.* Enter naphthalene.

- 0.20 days

4. Question: What chemical is CAS #110-75-8?

Answer: *Databases, Chemical, General Chemical Database, CAS number.* Enter number.

- 2-chloroethyl vinyl ether

5. Question: Under what condition would pentachlorophenol corrode rubber?

Answer: *Databases, Chemical, Specific Chemical Database, Choose Chemical.* Select pentachlorophenol. *Reactions, Corrosion.*

- When dissolved in oil

6. Question: What is the vapor density of 1,2-dichloropropane?

Answer: *Databases, Chemical, Specific Chemical Database, Choose Chemical.* Select dichloropropane. *1,2 isomers, Properties.*

- 3.9

7. Question: Who are the editors of a book containing information on the photodecomposition of ethylene dibromide?

Answer: Databases, *Chemical, Specific Chemical Database, Choose Chemical*. Select ethylene dibromide. *Reactions, Photochemical*.

To access the reference stack, click on the reference number (1311).

- Ramond E. Kirk, and Donald F. Othmer

8. Question: Is xylene carcinogenic?

Answer: Databases, *Chemical, Specific Chemical Database, Choose Chemical*. Select xylene. *Toxicology*.

- No

Hydrogeologic Database

Problem

Suppose a plastics manufacturer had buried drums of scrap material on their plant site in the past and recent fish kills in the river near the burial indicate there may be a leak. The site is located in the Gulf Coast region of Texas and the drums were buried in clayey loam underlain by a silty sand aquifer. The area is very swampy. You have the following field data for the aquifer:

Hydraulic conductivity = 10^{-3} cm/sec

Saturated thickness = 15 ft

Hydraulic gradient = .003 ft/ft

Depth to water = -5 ft

9. Question: Determine the region, the hydrogeologic setting, and the environment associated with this site.

Answer: Databases, *Hydrogeology, Begin: Access Database*.

- Region: *Atlantic and Gulf Coastal Plain*
- Setting: *Swamp*
- To see the hydrogeologic environment, click on *See Hydrogeologic Statistics*.
- Environment: *Sand and Gravel*

10. Question: What is the DRASTIC Index for this site?

Answer: After selecting the Region and the Setting for the site, click on. *Calculate Drastic Index*.

- 202; This index is high, which implies a high susceptibility to contamination.

11. Question: You are not sure about the accuracy of the hydraulic conductivity data that you obtained from the field. What is the mean and median values for the hydraulic conductivity found for sites similar to this?

Answer: After selecting the Region and the Setting for the site, click on *See Hydrogeologic Statistics*.

- mean = 0.0915 cm/s
- median = 0.008 cm/s

Modeling

Analytical model

Go to the analytical model section of OASIS by clicking on the words "Analytical Model" on the system flowchart. The first card shows ODAST, a 1-D analytical model. We hope to include others in a future version of the system. To see how the 1-D model works, read the help screen (? button) and run the example problem.

BIOPLUME II

Test Case 1: Create a plume

This test case involves only the BIOPLUME II section of OASIS. To begin, access the BIOPLUME II PreProcessor by clicking on "Preprocessor" in the system flowchart. You should now be on the first card of the stack titled "BIOPLUME II PreProcessor." Click the button in the lower left of the screen entitled "*New Users Click Here,*" then select "*Read This First*" to get crucial information about how the preprocessor works. The input data for a simple problem is listed below. Before entering any data, hit the "*Clear PreProcessor*" button on the right-hand side of the screen. Select "Yes" in the following dialog box which prompts you as follows, "Clear Previous Graphical Patterns?". If you cannot find the information on this sheet to fill in a blank, it is either not needed or can be entered using a default button on the appropriate card.

Configuration Card

Enter a grid size of 10 columns and 10 rows with cells of 60 x 60.

Note: The BIOPLUME II program adds a row (or column) of zeroes along each edge of the grid. Thus, the actual grid size will be 12 x 12 instead of 10 x 10.

Timing Parameters

One pumping period that lasts ten years and only one time step under steady state conditions. You may enter the rest of the information in this section or default.

Physical Parameters

Porosity = 0.3
Anisotropic ratio = 1.0
Longitudinal dispersivity = 10.0 ft
Ratio of transverse to longitudinal dispersivity = 0.3
Transmissivity = 0.001 ft²/s
Saturated thickness = 10.0 ft
Diffuse recharge = 0.0
No decay or aerobic degradation
Retardation factor = 1

Initial Conditions

Initial water table = 100
Initial contaminant conc = 0.0

Boundary Conditions

You have a row of constant heads of 100 at the top and 99.15 at the bottom and the direction of flow is north to south. You do not have any other constant head cells. You have an injection well at (5,3) with a rate of 2.47×10^{-6} cfs and a concentration of 15,000 mg/l. You do not have any area sources.

Numerical Parameters

Default

Run the model

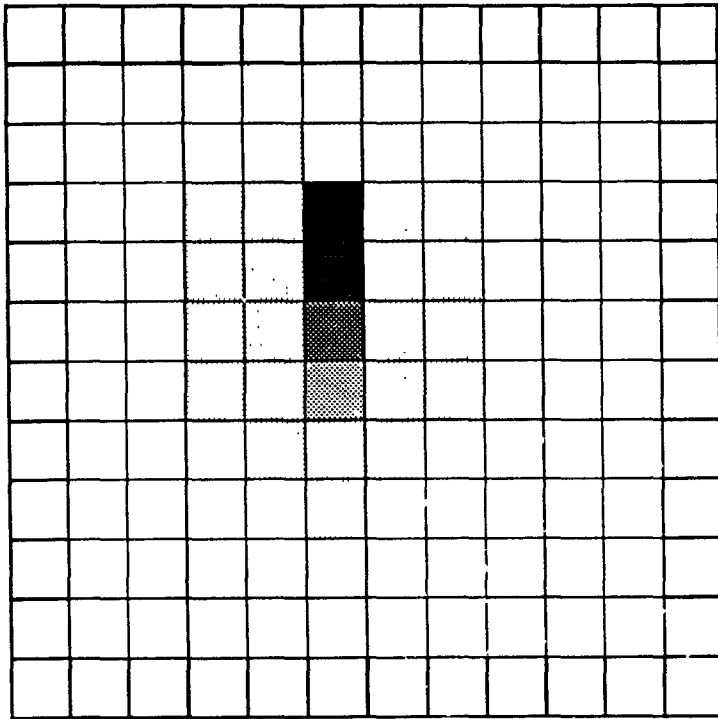
First, save your data to disk by hitting the "save to disk" button on the Preprocessor card. After hitting the "Save to Disk" button, you will see a standard save-file dialog box. This box allows you to decide where you would like to save your input file on the hard disk. If you have any questions about the procedure for saving a file, consult the Macintosh user's manuals. The system will also prompt you to enter a title for the file you are saving to disk. Please remember the location and name of the file you have just saved. The whole process will take around six minutes on an SE and about three minutes on a Mac II.

Once the data has been saved to disk, you are ready to run the model. Hit the "run the model" button on the Preprocessor card. After you have hit the "run the model" button, the system will ask you whether you are running on a Mac SE or a Mac II. After making the proper selection, the screen will go blank for a few seconds before a standard open-file dialog box appears on your screen. Select the folder in the dialog box which contains your input data set and open your input file. If you have any questions on the procedures for opening a file, please consult the Macintosh user's guide. The system will provide you with an output file name and BioGraph file name for your approval. Run time for the Trial 1 test problem is a little over three minutes on a Macintosh SE.











To run BioGraph, hit the "Run BioGraph" button on the first card of the preprocessor. Pull down the menu titled "file" and select "open" from the menu. Now open the BioGraph file you made when you ran the model (for example, Test Case 1. BioGraph). Pull down the "time" menu and select "forward" or "animate." BioGraph output is shown on the following page. For the output shown, the concentration limits for the patterns have been changed from the default limits set by BioGraph. For more detailed instructions, see the enclosed BioGraph User's Manual (Section 9.0).

To see the input or output file for your BIOPLUME II run, click the "View Data" button on the first card of the preprocessor. This button will open the Edit application. Click on the name of your input or output file to see the data.

Check your results with the results for test case, Trial 1, on the next page.



Legend : Values represent upper limits for corresponding pattern.

Concentration	
	1.00e-1
	3.25e+1
	6.49e+1
	9.74e+1
	1.30e+2
	1.62e+2
	1.95e+2
	2.27e+2
	2.60e+2
	2.92e+2

0 INPUT DATA
0 GRID DESCRIPTORS

NX (NUMBER OF COLUMNS) = 12
NY (NUMBER OF ROWS) = 12
XDEL (X-DISTANCE IN FEET) = 60.0
YDEL (Y-DISTANCE IN FEET) = 60.0

0 TIME PARAMETERS

NTIM (MAX. NO. OF TIME STEPS) = 1
NPMP (NO. OF PUMPING PERIODS) = 1
PINT (PUMPING PERIOD IN YEARS) = 10.000
TIMX (TIME INCREMENT MULTIPLIER) = .00
TINIT (INITIAL TIME STEP IN SEC.) = 0.

0 HYDROLOGIC AND CHEMICAL PARAMETERS

S (STORAGE COEFFICIENT) = .000000
POROS (EFFECTIVE POROSITY) = .300
BETA (LONGITUDINAL DISPERSIVITY) = 10.0
DLTRAT (RATIO OF TRANSVERSE TO
LONGITUDINAL DISPERSIVITY) = .30
ANFCTR (RATIO OF T-YY TO T-XX) = 1.000000

0 EXECUTION PARAMETERS

NITP (NO. OF ITERATION PARAMETERS) = 7
TOL (CONVERGENCE CRITERIA - ADIP) = .0010
ITMAX (MAX.NO.OF ITERATIONS - ADIP) = 200
CELDIS (MAX.CELL DISTANCE PER MOVE
OF PARTICLES - M.O.C.) = .500
NPMAX (MAX. NO. OF PARTICLES) = 9300
NPTPND (NO. PARTICLES PER NODE) = 9

1 PROGRAM OPTIONS
0

NPNT (TIME STEP INTERVAL FOR
COMPLETE PRINTOUT) = 1
NPNTMV (MOVE INTERVAL FOR CHEM.
CONCENTRATION PRINTOUT) = 0
NPNTVL (PRINT OPTION-VELOCITY
0=NO; 1=FIRST TIME STEP;
2=ALL TIME STEPS) = 0
NPNTD (PRINT OPTION-DISP.COEF.
0=NO; 1=FIRST TIME STEP;
2=ALL TIME STEPS) = 0
NUMOBS (NO. OF OBSERVATION WELLS
FOR HYDROGRAPH PRINTOUT) = 0
NREC (NO. OF PUMPING WELLS) = 1
NCODES (FOR NODE IDENT.) = 1
NPNCHV (PUNCH VELOCITIES) = 0
NPDELC (PRINT OPT. CONC. CHANGE) = 0

0 REACTION TERMS

DK (DISTRIBUTION COEFFICIENT) = 0.00000E+00
RHOB (BULK DENSITY OF SOLIDS) = 0.17500E+01
RF (RETARDATION FACTOR) = 0.10000E+01
THALF (HALF LIFE OF DECAY, IN SEC) = 0.00000E+00
DECAY (DECAY CONSTANT=LN 2/THALF) = 0.00000E+00

0 DECAY TERMS

DEC1 (ANAEROBIC DECAY COEFF.) = 0.00000E+00
DEC2 (REAERATION DECAY COEFF.) = 0.00000E+00

1 STEADY-STATE FLOW

TIME INTERVAL (IN SEC) FOR SOLUTE-TRANSPORT SIMULATION = 0.31558E+09

0 LOCATION OF PUMPING WELLS

X	Y	RATE(IN CFS)	CONC.	CONC(02)
6	4	-0.20E-05	15000.00	.00

0 AREA OF ONE CELL = 3600.

0 X-Y SPACING:

60.000
60.000

1TRANSMISSIVITY MAP (FT*FT/SEC)

0.00E-01	0.00E-01	0.00E-01	0.00E-01	0.00E-01	0.00E-01	0.00E-01	0.00E-01	0.00E-01	0.00E-01
0.00E-01	0.00E-01								
0.00E-01	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03
1.00E-03	0.00E-01								
0.00E-01	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03
1.00E-03	0.00E-01								
0.00E-01	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03
1.00E-03	0.00E-01								
0.00E-01	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03
1.00E-03	0.00E-01								
0.00E-01	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03
1.00E-03	0.00E-01								

1AQUIFER THICKNESS (FT)

1DIFFUSE RECHARGE AND DISCHARGE (FT/SEC)

1PERMEABILITY MAP (FT/SEC)

0 NO. OF FINITE-DIFFERENCE CELLS IN AQUIFER = 100

```
NZCRIT (MAX. NO. OF CELLS THAT CAN BE VOID OF
        PARTICLES; IF EXCEEDED, PARTICLES ARE REGENERATED) = 2
```

[illegible]

[illegible][illegible]

```

NUMBER OF TIME STEPS =      0
TIME(SECONDS) =      .00000
TIME(DAYS) =      0.00000E+00
TIME(YEARS) =      0.00000E+00

```

```

1 ITERATION PARAMETERS
0.171347E-01
0.337467E-01
0.664638E-01
.130900
.257806
.507746
1.00000
.000000
.000000

```



```

0      0      1      1      1      1      1      1      1      1      1      1      0
0      0      1      1      1      1      1      1      1      1      1      1      0
0      0      1      1      1      1      1      1      1      1      1      1      0
0      0      0      0      0      0      0      0      0      0      0      0      0
0      0      0      0      0      0      0      0      0      0      0      0      0
0 CUMULATIVE MASS BALANCE -- (IN FT**3)

RECHARGE AND INJECTION      = -0.63115E+03
PUMPAGE AND E-T WITHDRAWAL = 0.00000E+00
CUMULATIVE NET PUMPAGE      = -0.63115E+03
WATER RELEASE FROM STORAGE = 0.00000E+00
LEAKAGE INTO AQUIFER        = 0.29709E+06
LEAKAGE OUT OF AQUIFER      = -0.29793E+06
CUMULATIVE NET LEAKAGE      = -0.84691E+03
0   MASS BALANCE RESIDUAL    = -215.75
    ERROR (AS PERCENT)      = -0.72442E-01

0 RATE MASS BALANCE -- (IN C.F.S.)

LEAKAGE INTO AQUIFER        = 0.94141E-03
LEAKAGE OUT OF AQUIFER      = -0.94409E-03
NET LEAKAGE (QNET)          = -0.26835E-05
RECHARGE AND INJECTION      = -0.20000E-05
PUMPAGE AND E-T WITHDRAWAL = 0.00000E+00
NET WITHDRAWAL (TPUM)       = -0.20000E-05
1   STABILITY CRITERIA --- M.O.C.

0   FLUID VELOCITIES
VMAX = 2.09E-09      VMAY = 5.30E-07
VMXBD= 2.85E-09      VMYBD= 5.32E-07
0   TIMV (MAX. INJ.) = 0.11446E+09
    TIMV (CELDIS)    = 0.56389E+08
0   TIMV = 5.64E+07      NTIMV = 5      NMOV = 6

    TIM (N) = 0.31558E+09
    TIMEVELO = 0.52596E+08
    TIMEDISP = 0.26073E+09
0   TIMV = 5.26E+07      NTIMD = 1      NMOV = 6
0   THE LIMITING STABILITY CRITERION IS CELDIS
0   NO. OF PARTICLE MOVES REQUIRED TO COMPLETE THIS TIME STEP = 6

0   NP      = 1151      IMOV      = 1
    TIM(N)   = 0.31558E+09      TIMV      = 0.52596E+08      SUMTCH = 0.52596E+08
0   NP      = 1157      IMOV      = 2
    TIM(N)   = 0.31558E+09      TIMV      = 0.52596E+08      SUMTCH = 0.10519E+09
0   NP      = 1157      IMOV      = 3
    TIM(N)   = 0.31558E+09      TIMV      = 0.52596E+08      SUMTCH = 0.15779E+09
0   NP      = 1166      IMOV      = 4
    TIM(N)   = 0.31558E+09      TIMV      = 0.52596E+08      SUMTCH = 0.21038E+09
0   NP      = 1184      IMOV      = 5
    TIM(N)   = 0.31558E+09      TIMV      = 0.52596E+08      SUMTCH = 0.26298E+09
0   NP      = 1193      IMOV      = 6
    TIM(N)   = 0.31558E+09      TIMV      = 0.52596E+08      SUMTCH = 0.31558E+09
1 CONCENTRATION OF CONTAMINANT

NUMBER OF TIME STEPS = 1
DELTA T              = 0.31558E+09
TIME (SECONDS)       = 0.31558E+09
CHEM.TIME (SECONDS)  = 0.31558E+09
CHEM.TIME (DAYS)     = 0.36525E+04
TIME (YEARS)         = 0.10000E+02
CHEM.TIME (YEARS)    = 0.10000E+02
NO. MOVES COMPLETED = 6

0   0   0   0   0   0   0   0   0   0   0   0   0
0   0   0   0   0   0   0   2   0   0   0   0   0
0   0   0   0   0   0   1   25   1   0   0   0   0
0   0   0   0   0   0   9   292   9   0   0   0   0
0   0   0   0   0   1   16   247   16   1   0   0   0
0   0   0   0   0   0   14   179   14   0   0   0   0
0   0   0   0   0   0   5   78   5   0   0   0   0
0   0   0   0   0   0   1   13   1   0   0   0   0
0   0   0   0   0   0   0   1   0   0   0   0   0
0   0   0   0   0   0   0   0   0   0   0   0   0
0   0   0   0   0   0   0   0   0   0   0   0   0
0   0   0   0   0   0   0   0   0   0   0   0   0
0   0   0   0   0   0   0   0   0   0   0   0   0

CHEMICAL MASS BALANCE

MASS IN BOUNDARIES      = 0.00000E+00
MASS OUT BOUNDARIES     = -0.27079E+02
MASS PUMPED IN           = 0.94673E+07
MASS PUMPED OUT          = -0.00000E+00
MASS LOST W. BIODEG.     = 0.21958E-02
MASS LOST BY RADIO. DCY= 0.00000E+00
MASS LOST BY ANAER. DCY= 0.00000E+00
MASS LOST BY REAER. DCY= 0.00000E+00
MASS ADSORBED ON SOLIDS= 0.00000E+00
INITIAL MASS ADSORBED    = 0.00000E+00

```



```
INFLOW MINUS OUTFLOW = 0.94673E+07
INITIAL MASS DISSOLVED = 0.00000E+00
PRESENT MASS DISSOLVED = 0.10092E+08
CHANGE MASS DISSOLVED = 0.10092E+08
CHANGE TOTL.MASS STORED= 0.10092E+08
COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
MASS BALANCE RESIDUAL = -0.62455E+06
ERROR (AS PERCENT) = -0.65970E+01
1Trial1
```


0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0

9.0

BioGraph

*Graphical Analysis
for
Bioplume II*

by John F. Haasbeek

June 1989

9.0 DESCRIPTION OF THE PROGRAM

The goal of the BioGraph program is to facilitate the examination of output from the BIOPLUME model and to present as much of the output information in a graphical manner as is possible. The program is fully interactive and is controlled by mouse operations. It centers around the display of output variables such as contaminant and oxygen concentrations using patterns to represent the output graphically on a grid. In addition, the program provides several tools with which the user can view the data in many ways.

The input files for the program are written by the BIOPLUME model. Each time the model is run, it writes a duplicate set of output to a file. You specify the name for this file when you run the model. Please note that at this time the BioGraph program can only display data from a steady-state BIOPLUME run for one pumping period only. In addition, the head map should only be written for the first time step. These restrictions are present to simplify the development process and will be removed at a later stage.

If you get a system error while reading an input file, especially error number 16, this means that the file you have selected is not correctly formatted. Restart the computer and re-run the BIOPLUME model making sure you have followed the above restrictions.

Starting

You can transfer to BioGraph from the Model Options card, from the system outline, or from the preprocessor. When the program begins, you will see a large blank window and several menus. This window is referred to as the main window, and this is where the grid patterns are displayed. Program operation is controlled by commands located in pull-down menus. The first step in using BioGraph is to open a BIOPLUME output file. The command to do this is located in the **File** menu and is called **Open**. Selecting this command will allow you access to the standard file selection dialog. If you do not know how to use this to locate the file you are looking for, please read the Macintosh user's manual supplied with your computer. Once a file has been opened, the program will read in the data and display initial contaminant concentrations in the main window. When the cursor is over the grid, the cell coordinates and the cell value are displayed at the top of the grid. Other variables can be displayed, and mouse clicks within the grid access graphs versus time or distance. The operation of the program is described below as each of the commands are listed and explained. Remember, the best way to see what a command does is to try it.

Menus

In this section, the menus are described and each command is explained. Many of the menu commands have keyboard equivalents - these are described under the Open command. Note that these are all of the program commands - everything the program does is accessible through menu commands.

Apple Menu

The first menu in the menu area is the **Apple** menu. It allows access to all desk accessories installed in the system and also includes the "**About BioGraph ...**" command.

File Menu

The **File** menu contains commands which control the general operation of the program.

The "**Open**" command brings up the standard file selection box, from which you can select an input file for BioGraph. Most of the other menu commands will be dimmed (and thus inaccessible) until you have selected an input file. The cloverleaf symbol followed by a letter at the right of a command indicates that a keyboard command exists which is equivalent to choosing that command from the menu. The apple/cloverleaf symbol represents the Command key or Control key on the keyboard. For example, a shortcut for opening files is to hold down the Command/Control key and type "o." There are many keyboard shortcuts included in the menus.

The "**Options**" command allows you to set various options for program operation. These include animation speed and graph scaling. To change an option, simply check the corresponding box. Once the options are set, click the button marked OK.

The "**Calibration Data**" command is currently disabled, pending further review.

"**Print Plume**," as the name implies, allows you to print the plume on any attached printer. There are three dialog boxes associated with printing: the first requests the printing scale in terms of cell length in inches. Thus, if you have a model cell size of 50 feet on a side, you would specify 0.25 to print at 1":200'. The next two dialogs are the standard Macintosh printing dialog boxes.

Also, you may hit *command - shift - 3* to save a copy of the current screen as a picture file. The saved files will be named sequentially Screen0 through Screen9 and will be found on the desktop. Any paint program will open the saved picture file and allow you to edit the picture.

The "**Quit**" command exits the program.

Modes Menu

When the model grid is displayed in the main window, the program operates in one of three modes. These modes are selected by the corresponding command in the "**Modes**" menu. The cursor shape indicates which mode you are in as well as a check mark in the menu next to the current mode. In Time mode, a mouse click in a grid cell calls up a graph of the current variable versus time in that cell. The current variable depends on what is currently being displayed in the grid - see the "**Windows**" menu. This option has no effect while displaying heads unless the file contains data from a transient run. In the Options dialog, you may choose if you want both oxygen and contaminant graphs to appear for each mouse click.

The Distance mode is different from the Time mode in that it requires two grid cells for input. Graphs of concentrations or heads are then drawn as a cross section between the two grid cells at the current time step. The grid cells which will comprise the ends of the cross section are selected by pressing the mouse button down in the first grid cell, dragging the cursor to the second grid cell keeping the mouse button down, and then releasing the button over the second cell. Note that the cells must form a horizontal or vertical line. Again, you may choose in the Options dialog whether to display both contaminant and oxygen cross sections or only the current variable. Note also that while the cross sections are displayed, you may change time step (see **Time** menu) and the graphs will automatically be updated.

In Both mode, you select a cross section in the same manner as described above, but when the graphs appear, cross sections are drawn for each time step.

The last two options in this menu, **Patterns** and **Contours**, toggle between the corresponding display modes. Use these commands to select display of patterns or contours representing data in the grid. Note that the contour display routine is still very much under development, and so is not perfect. If you switch to contours, you will probably want to set the contour values differently than the pattern limits. The commands to do this are in the rightmost menu. The rightmost menu title will be "Patterns" when in pattern mode and "Contours" when in contour mode.

Time Menu

The Time menu is used to control which time step is being displayed. In the main window and the various graph windows, data is displayed for the current time step. If you wish to display data for the next time step, simply choose "**Forward.**" Similarly, to display data for the previous time step, choose "**Backward.**" The "**Animate**" command displays all data sequentially starting at the first time step. You may adjust animation speed in the Options dialog.

Windows Menu

The **Windows** menu contains commands which control what is to be displayed in the main window, and consequently which is the "current" variable. The "**Contaminant,**" "**Oxygen,**" and "**Head Map**" commands select the corresponding variable for display. The "**Base Map**" and "**Combined**" commands are currently disabled.

Other Info Menu

The Other Info menu contains only one command. This command, "**Mass Balance,**" is also currently disabled.

Color Menu

The Color menu only appears when the program is running on a Mac II. It allows you to select a color for the main window display. The currently selected color has a check mark next to it.

Patterns Menu

Each pattern represents concentrations or head values less than or equal to a certain limit. These are set by default by the program when input is read, but you can set the limits through the **Limits** command in the **Patterns** menu. When selected, a dialog box will appear in which you may fill in limits of your choice. Click Cancel to return to the previous pattern limits.

Contours Menu

The default contour values are the current pattern limits. To change them (which you will definitely want to do to see nice contours) use the **Intervals** command in the **Contours** menu. The method is the same as for changing pattern limits; however, the numbers now represent values to contour. Note - 0 is a bad number to contour. To see the edge of the plume, contour a concentration of 1 or 0.1. If you set the highest contour to 0.1 and all the others to -1, you will get a single contour of the edge of the plume. This will make for fast contouring over time. The **Sequence** command creates a snapshot of the contour picture for each time step and records them in a sequence. Every time you select this command after the first, the sequence will be played back, saving lots of time. The sequence will have to be redrawn if you change window sizing or contour values, etc.

10.0 REFERENCES

- Aller, L., T. Bennett, J. Lehr, R. J. Petty, and G. Hackett. 1987. DRASTIC: A Standardized System for Evaluating Ground Water Pollution Potential Using Hydrogeologic Settings. U.S. EPA. EPA-600/2-87-035.
- Javandel L., C. Doughty, C. F. Tsang. 1984. Groundwater Transport: Handbook of Mathematical Models. American Geophysical Union, Washington, DC.
- Konikow, L. F. and Bredehoeft, J. D. 1978. Computer model of two-dimensional solute transport and dispersion in ground water. In: Automated Data Processing and Computations, Techniques of Water Resources Investigations.
- McClymont, G.L. and F. W. Schwartz. 1987. Development and Application of an Expert System in Contaminant Hydrogeology: The Expert ROKEY System. National Hydrology Research Institute. DSS File No.: 52SS. KN107-5-4334. Serial No.: OSS85-00149.
- Newell, C.J., L.P. Hopkins, and P.B. Bedient. 1988. Hydrogeologic Database for Ground Water Modeling. Report for the American Petroleum Institute.
- Newell, C. J., J. F. Haasbeek and P. B. Bedient. Accepted for March 1990. OASIS: A Graphical Decision Support System for Ground Water Contamination Modeling. Groundwater.
- Rifai, H. S., P. B. Bedient, J. T. Wilson, K. M. Miller, and J. M. Armstrong. 1988. Biodegradation Modeling at a Jet Fuel Spill Site. J. Environmental Engineering Division, ASCE Environmental Engineering Division. Vol. 114, No. 5, pp 1007-1028.

SOFTWARE DISCLAIMER

"APPLE COMPUTER, INC. ("APPLE") MAKES NO WARRANTIES, EXPRESS OR IMPLIED, INCLUDING WITHOUT LIMITATION THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE, REGARDING THE APPLE SOFTWARE. APPLE DOES NOT WARRANT, GUARANTEE OR MAKE ANY REPRESENTATIONS REGARDING THE USE OR THE RESULTS OF THE USE OF THE APPLE SOFTWARE IN TERMS OF ITS CORRECTNESS, ACCURACY, RELIABILITY, CURRENTNESS OR OTHERWISE. THE ENTIRE RISK AS TO THE RESULTS AND PERFORMANCE OF THE APPLE SOFTWARE IS ASSUMED BY YOU. THE EXCLUSION OF IMPLIED WARRANTIES IS NOT PERMITTED BY SOME STATES. THE ABOVE EXCLUSION MAY NOT APPLY TO YOU."

Developer shall also include the following disclaimer of liability language in the same place:

"IN NO EVENT WILL APPLE, ITS DIRECTORS, OFFICERS, EMPLOYEES OR AGENTS BE LIABLE TO YOU FOR ANY CONSEQUENTIAL, INCIDENTAL OR INDIRECT DAMAGES (INCLUDING DAMAGES FOR LOSS OF BUSINESS PROFITS, BUSINESS INTERRUPTION, LOSS OF BUSINESS INFORMATION, AND THE LIKE) ARISING OUT OF THE USE OR INABILITY TO USE THE APPLE SOFTWARE EVEN IF APPLE HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES. BECAUSE SOME STATES DO NOT ALLOW THE EXCLUSION OR LIMITATION OF LIABILITY FOR CONSEQUENTIAL OR INCIDENTAL DAMAGES, THE ABOVE LIMITATIONS MAY NOT APPLY TO YOU. Apple's liability to you for actual damages from any cause whatsoever, and regardless of the form of the action (whether in contract, tort (including negligence), product liability or otherwise), will be limited to \$50."